Convexity of the phase boundary in the BCS model with imaginary magnetic field

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Abstract

We study geometric properties of the domain of the two parameters (inverse temperature, imaginary magnetic field) where the gap equation of the BCS model with imaginary magnetic field has a positive solution. If the interaction is weak and the free dispersion relation is non-vanishing, the domain is a disjoint union of periodic copies of one representative set in the plane of (inverse temperature, imaginary magnetic field). In this paper we provide a necessary and sufficient condition for the representative set to be convex as the main result. More precisely we prove the following. The representative set is convex for any weak coupling and non-vanishing free dispersion relation if and only if the minimum of the magnitude of the free dispersion relation over the maximum is larger than the critical value $\sqrt{9-4\sqrt{5}}$. In the context of dynamical quantum phase transition (DQPT) the imaginary magnetic field is considered as the real time variable. So this is an analysis of the phase boundary of a DQPT in the plane of (inverse temperature, real time). In particular convexity of the representative phase boundary is characterized by the critical constant $\sqrt{9-4\sqrt{5}}$. The gap equation rigorously derived in the preceding paper [Y. Kashima, J. Math. Sci. Univ. Tokyo **28** (2021), 399–556] is at the core of our analysis. *

1 Introduction and main results

1.1 Introduction

It is an interesting subject to study the Bardeen-Cooper-Schrieffer (BCS) model, which has been a paradigm of describing phase transitions, in non-equilibrium setting. In recent years a non-equilibrium phenomenon called dynamical quantum phase transition (DQPT) has been actively investigated. DQPTs are defined by

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non-analyticity of a dynamical analogue of the free energy density with the real time variable ([9], [7]). It emerged that the BCS model with imaginary magnetic field introduced in [11], [12], [13] can naturally fit in the formalism of DQPT at positive temperature. This connection motivates us to reveal universal properties of this non-Hermitian system.

Let us explain more about the link between the BCS model with imaginary magnetic field and the concept of DQPT. Let H, S_z denote the BCS model with the reduced BCS interaction, the z-component of the spin operator respectively. These operators will be defined explicitly in Subsection 1.2. We want to know where the following function loses analyticity in $\mathbb{R}_{>0} \times \mathbb{R}$.

$$(\beta, t) \mapsto \lim_{N\to\infty} \left(-\frac{1}{\beta N} \log(\mathrm{Tr}\, e^{-\beta \mathsf{H} + it\mathsf{S}_z}) \right). \tag{1.1}$$

Here β is the inverse temperature and N denotes the system size. We are calling the complex number it ($t \in \mathbb{R}$) imaginary magnetic field for convenience. The real variable t can be considered as real time in the context of DQPT as explained below. Since the right-hand side of (1.1) can formally be seen as the free energy density of the BCS model interacting with the imaginary magnetic field, we call the loss of analyticity of the function (1.1) phase transition by analogy with the conventional definition of phase transition. In this paper as in our previous work [11], [12], [13], [14] the BCS interaction is assumed to be weak, and thus there is no phase transition defined by non-analyticity of the free energy density without the imaginary magnetic field

$$\beta \mapsto \lim_{N\to\infty} \left(-\frac{1}{\beta N} \log(\mathrm{Tr}\, e^{-\beta \mathsf{H}}) \right).$$

Therefore the regularity of the function (1.1) is the same as that of

$$(\beta, t) \mapsto \lim_{N\to\infty} \left(-\frac{1}{\beta N} \log\left(\frac{\mathrm{Tr}\, e^{-\beta \mathsf{H} + it\mathsf{S}_z}}{\mathrm{Tr}\, e^{-\beta \mathsf{H}}} \right) \right).$$

Since H commutes with S_z,

$$e^{-\beta \mathsf{H} + it\mathsf{S}_z} = e^{-\beta \mathsf{H}} e^{it\mathsf{S}_z} = e^{-\beta \mathsf{H}} e^{-it\mathsf{H}} e^{it(\mathsf{H}+\mathsf{S}_z)}.$$

We conclude that the regularity of (1.1) is the same as that of

$$(\beta, t) \mapsto \lim_{N\to\infty} \left(-\frac{1}{\beta N} \log\left(\frac{\mathrm{Tr}(e^{-\beta \mathsf{H}} e^{it\mathsf{S}_z})}{\mathrm{Tr}\, e^{-\beta \mathsf{H}}} \right) \right), \tag{1.2}$$

$$(\beta, t) \mapsto \lim_{N\to\infty} \left(-\frac{1}{\beta N} \log\left(\frac{\mathrm{Tr}(e^{-\beta \mathsf{H}} e^{-it\mathsf{H}} e^{it(\mathsf{H}+\mathsf{S}_z)})}{\mathrm{Tr}\, e^{-\beta \mathsf{H}}} \right) \right) \tag{1.3}$$

in $\mathbb{R}_{>0} \times \mathbb{R}$. The function (1.2) can be considered as the finite-temperature version of the rate function of the Loschmidt amplitude $\langle \psi_0, e^{it\mathsf{S}_z} \psi_0 \rangle$, where ψ_0 is the ground state of H. The appearance of non-analyticity of the function (1.2) with the time t defines DQPT. This definition is in line with e.g. [3], [8], [16]. On the other hand, according to [23], [21], the characteristic function of the work done in the many-electron system by suddenly changing the initial Hamiltonian H to $\mathsf{H} + \mathsf{S}_z$ is given by

$$\frac{\mathrm{Tr}(e^{-\beta \mathsf{H}} e^{-it\mathsf{H}} e^{it(\mathsf{H}+\mathsf{S}_z)})}{\mathrm{Tr}\, e^{-\beta \mathsf{H}}}. \tag{1.4}$$

Based on this observation, DQPT is defined by non-analyticity of the function (1.3) with t. This alternative definition appears in e.g. [1], [17], [20]. As explained in [21], (1.4) is also considered as the finite-temperature version of the Loschmidt amplitude $\langle\psi_0, e^{-it\mathsf{H}}e^{it(\mathsf{H}+\mathsf{S}_z)}\psi_0\rangle$. So the variable t can be interpreted as real time in this definition as well. We can now see that studying properties of (1.1) is relevant to the recent physical research of DQPT, though the papers [3], [8], [16], [1], [17], [20] treat 1D quantum spin systems and 2D non-interacting Fermion systems as benchmark models. In this paper we aim at characterizing the phase boundary where the function (1.1) loses analyticity geometrically. In other words our purpose is to characterize the phase boundary of DQPT in the plane of (inverse temperature, real time).

For clarity we remark that it is not common at present to draw a phase boundary with the real time axis as we do in this paper. In the physics literature on DQPT what is called dynamical phase diagrams are drawn with other control parameters for which a dynamical analogue of the free energy density shows non-analytic behavior with time. See e.g. [25], [6], [16].

In order to explain the main result of this paper in more detail, let us recall what have been proved in the BCS model with imaginary magnetic field so far. It was proved in the preceding papers [11], [12], [13] that transitions between the normal phase and the superconducting phase occur at positive temperature. In the plane of (β, t) the superconducting phase is a domain where the gap equation has a positive solution $\Delta(\beta, t)$, which we call gap function or order parameter. In [11], [12] where the free Fermi surface is non-empty the possible magnitude of the BCS interaction depends on the temperature and the imaginary magnetic field. In [13] where the free Fermi surface is empty or in other words the free dispersion relation is non-vanishing the interaction must still be small. However, the magnitude can be independent of the temperature and the imaginary magnetic field. This enables us to fully draw the phase boundary on the plane of (inverse temperature, imaginary magnetic field) or equivalently (inverse temperature, real time) for any sufficiently small BCS coupling and study its geometric properties while justifying the derivation of the gap equation. In [13, Section 2] we saw that the phase boundary is a disjoint union of periodic copies of one representative simple curve and the upper half of the representative curve is the reflection of its lower half across a horizontal line. To understand the situation with non-vanishing free dispersion relation better, we remark the following relations. Here $p(\in \mathbb{R}_{>0})$ denotes a period.

(1.5)

$$
\begin{aligned}
&\text{(Phase boundary)}\\
&\;= \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \text{the function (1.1) is not analytic at } (\beta, t)\}\\
&\;= \text{Boundary of } \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \text{the gap equation has a positive solution } \Delta(\beta, t)\}\\
&\qquad \cap\, \mathbb{R}_{>0} \times \mathbb{R}\\
&\;= \bigsqcup_{m\in\mathbb{Z}} \{(\beta, t + pm) \mid (\beta, t) \in \text{(the representative simple curve)}\},\\
&\text{(the representative simple curve)} = \text{(the lower half)} \cup \text{(the upper half)},\\
&\text{(the upper half)} = \text{(reflection of the lower half across a horizontal line)},
\end{aligned}
$$

(1.6)

$$\{(\beta,t)\in\mathbb{R}_{>0}\times\mathbb{R}\mid \text{the gap equation has a positive solution } \Delta(\beta,t)\}$$
$$=\bigsqcup_{m\in\mathbb{Z}}\{(\beta,t+pm)\mid(\beta,t)\in(\text{the representative set})\},$$
$$\text{Boundary of (the representative set)}\cap\mathbb{R}_{>0}\times\mathbb{R}$$
$$=(\text{the representative simple curve}).$$

Therefore it is sufficient to focus on the lower half of the representative curve to analyze the whole phase boundary.

To simplify subsequent explanations, let e_{min}, e_{max} ($0 < e_{min} \le e_{max}$) denote the minimum, the maximum of the magnitude of a non-vanishing free dispersion relation respectively. These will be rigorously defined in Subsection 1.2.

In this paper we continue working on the BCS model whose free dispersion relation is non-vanishing under the influence of imaginary magnetic field at positive temperature. As explained above, the set $\{(\beta,t)\in\mathbb{R}_{>0}\times\mathbb{R}\mid\Delta(\beta,t)>0\}$ is a disjoint union of periodic copies of one representative set of (β,t), whose boundary is the representative simple curve. We prove the following statement as the main result. The representative set is convex for any non-vanishing free dispersion relation having e_{min}, e_{max} and any weak coupling constant if and only if $\frac{e_{min}}{e_{max}}$ is larger than the critical value $\sqrt{9-4\sqrt{5}}$.

Since the upper half of the representative simple curve is the reflection of the lower half, the convexity of the representative set is equivalent to the convexity of the lower half of the representative curve. The main results of [13, Section 2], [14] and this paper can be summarized in terms of geometric properties of the lower half of the representative curve of the phase boundary as follows.

- In [13, Theorem 2.19] the unique existence of a local minimum point is characterized by the relation between $\frac{e_{min}}{e_{max}}$ and the critical constant $\sqrt{17-12\sqrt{2}}$.
- In [14, Theorem 1.7, Theorem 1.8] the (non-)existence of a stationary point of inflection is characterized by the relation between $\frac{e_{min}}{e_{max}}$ and the critical constant $\sqrt{17-12\sqrt{2}}$.
- In Theorem 1.11 of this paper the convexity is characterized by the relation between $\frac{e_{min}}{e_{max}}$ and the critical constant $\sqrt{9-4\sqrt{5}}$.

A more rigorous version of the summary is given in Remark 1.15. Since the convexity implies the uniqueness of a local minimum point and $\sqrt{9-4\sqrt{5}}(\approx 0.236068) > \sqrt{17-12\sqrt{2}}(\approx 0.171573)$, the stronger property of the phase boundary is characterized by the stronger inequality $\frac{e_{min}}{e_{max}} > \sqrt{9-4\sqrt{5}}$ in Theorem 1.11 than in [13, Theorem 2.19]. We are interested in the fact that various fundamental properties of the phase boundary can be systematically characterized by the relation between $\frac{e_{min}}{e_{max}}$ and the critical constants. This is the mathematical motivation behind this series. We add that existence of a stationary point of inflection is equivalent to existence of a higher order phase transition with temperature, and thus [14, Theorem 1.7, Theorem 1.8] characterize the (non-)existence of a higher order phase transition with temperature as well.

We focus on a class of non-vanishing free dispersion relations mainly because the derivation of the gap equation from the many-Fermion system is justified for any temperature and imaginary magnetic field. DQPTs in insulating Hamiltonians with ground state topology are a central topic in the research area. Some of the benchmark models can be written with one-particle Hamiltonian matrices belonging to our class. These are e.g. the Haldane model ([5], [8]), the Su-Schrieffer-Heeger model ([22], [10]). Concrete construction of these models with our notations was given in [14, Remark 1.2]. It is encouraging that our class of non-vanishing free dispersion relations is relevant to the recent research of DQPT.

There are technically close relations between [13, Section 2] and [14]. The previous work [14] applies some key lemmas established in [13, Section 2]. In this paper we admit the gap equation derived in [13]. We also have a few simple lemmas in common with [13, Section 2], [14]. However, the technical construction is essentially different from these preceding papers. Key lemmas necessary to prove the main results are newly established here. In this sense this paper is more self-contained than [14].

We do not find a research article on DQPT in the BCS model at positive temperature, apart from [11], [12], [13], [14] at present. Concerning DQPTs in the BCS model at zero temperature, we cite the recent paper [19]. Though only a few articles report on DQPT in the BCS model so far, there are many papers on non-equilibrium phases characterized by long time behavior of the dynamical order parameter of the model. See e.g. the references of [19] or [18], [24]. The paper [19] investigates whether the DQPT can indicate these non-equilibrium phases defined differently.

This paper is outlined as follows. In the next subsection we set up notations and state the main results. In Section 2 we prove that if $\frac{e_{min}}{e_{max}} > \sqrt{9-4\sqrt{5}}$, the representative set of the domain where the gap function is positive is convex for any sufficiently small coupling constant. In Section 3 we prove that if $\frac{e_{min}}{e_{max}} < \sqrt{9-4\sqrt{5}}$, the convexity of the representative set does not necessarily hold. Finally in Section 4 we show that if $\frac{e_{min}}{e_{max}} = \sqrt{9-4\sqrt{5}}$, the convexity does not necessarily hold, either. This completes the characterization of the convexity in terms of the relation between $\frac{e_{min}}{e_{max}}$ and the critical constant $\sqrt{9-4\sqrt{5}}$.

1.2 Notations and the main results

Here we introduce necessary notations and state the main results. We are going to analyze the phase boundary, which is governed by the gap equation. The gap equation was originally derived from a many-electron system in [13]. Though we do not explain the derivation in detail, it must be informative to present the corresponding many-electron system explicitly. Let the number $d(\in \mathbb{N})$ denote the spatial dimension. Let $\mathbf{v}_1, \cdots, \mathbf{v}_d$ be a basis of $\mathbb{R}^d$ and $\hat{\mathbf{v}}_1, \cdots, \hat{\mathbf{v}}_d$ be its dual basis. Let b, $L \in \mathbb{N}$. We consider a general spatial lattice which has b sites in its unit cell. Such a lattice can be identified as $\mathcal{B} \times \Gamma$, where $\mathcal{B} := \{1, \cdots, b\}$,

$$\Gamma := \left\{ \sum_{j=1}^{d} m_j \mathbf{v}_j \ \middle|\ m_j \in \{0, 1, \cdots, L-1\} \ (j = 1, \cdots, d) \right\}.$$

The momentum lattice dual to $\mathcal{B} \times \Gamma$ is $\mathcal{B} \times \Gamma^*$, where

$$\Gamma^* := \left\{ \sum_{j=1}^{d} \hat{m}_j \hat{\mathbf{v}}_j \ \middle|\ \hat{m}_j \in \left\{0, \frac{2\pi}{L}, \cdots, \frac{2\pi}{L}(L-1)\right\} \ (j = 1, \cdots, d) \right\}.$$

The free Hamiltonian H_0 is defined by

$$\mathsf{H}_0 := \sum_{\substack{(\rho,\mathbf{x}),(\eta,\mathbf{y}) \\ \in \mathcal{B}\times\Gamma}} \sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{\mathbf{k}\in\Gamma^*} e^{i\langle \mathbf{k},\mathbf{x}-\mathbf{y}\rangle} E(\mathbf{k})(\rho,\eta)\psi^*_{\rho\mathbf{x}\sigma}\psi_{\eta\mathbf{y}\sigma}, \tag{1.7}$$

where $\langle\cdot,\cdot\rangle$ denotes the standard inner product of $\mathbb{R}^d$ and $\psi^*_{\rho\mathbf{x}\sigma}$, $\psi_{\rho\mathbf{x}\sigma}$ ($(\rho,\mathbf{x},\sigma) \in \mathcal{B}\times\Gamma\times\{\uparrow,\downarrow\}$) denote the creation, the annihilation operator on the Fermionic Fock space $F_f(L^2(\mathcal{B}\times\Gamma\times\{\uparrow,\downarrow\}))$ respectively. The matrix-valued function $E : \mathbb{R}^d \to \mathrm{Mat}(b,\mathbb{C})$ plays an important role in this paper. We call it one-particle free Hamiltonian matrix and its eigenvalues parameterized by the momentum variable $\mathbf{k}$ free dispersion relations. With constants e_{min}, $e_{max} \in \mathbb{R}_{>0}$ satisfying $e_{min} \le e_{max}$ we define the set $\mathcal{E}(e_{min}, e_{max})$ of one-particle free Hamiltonian matrices as follows. $E \in \mathcal{E}(e_{min}, e_{max})$ if and only if

$$\begin{aligned}
&E \in C^\infty(\mathbb{R}^d, \mathrm{Mat}(b,\mathbb{C})), && (1.8)\\
&E(\mathbf{k}) = E(\mathbf{k})^*,\ \forall \mathbf{k}\in\mathbb{R}^d,\\
&E(\mathbf{k}+2\pi\hat{\mathbf{v}}_j) = E(\mathbf{k}),\ \forall\mathbf{k}\in\mathbb{R}^d,\ j\in\{1,\cdots,d\},\\
&E(\mathbf{k}) = \overline{E(-\mathbf{k})},\ \forall\mathbf{k}\in\mathbb{R}^d, && (1.9)\\
&\inf_{\mathbf{k}\in\mathbb{R}^d} \inf_{\substack{\mathbf{u}\in\mathbb{C}^b \\ \text{with } \|\mathbf{u}\|_{\mathbb{C}^b}=1}} \|E(\mathbf{k})\mathbf{u}\|_{\mathbb{C}^b} = e_{min}, && (1.10)\\
&\sup_{\mathbf{k}\in\mathbb{R}^d} \|E(\mathbf{k})\|_{b\times b} = e_{max}. && (1.11)
\end{aligned}$$

Here $\|\cdot\|_{\mathbb{C}^b}$ is the standard norm of $\mathbb{C}^b$ induced by the Hermitian inner product and $\|\cdot\|_{b\times b}$ is the operator norm on $\mathrm{Mat}(b,\mathbb{C})$. Here we consider $\mathrm{Mat}(b,\mathbb{C})$ as a Banach space with the norm $\|\cdot\|_{b\times b}$ and $C^\infty(\mathbb{R}^d, \mathrm{Mat}(b,\mathbb{C}))$ as the set of the Banach space valued smooth functions. In fact the smoothness (1.8) can be relaxed and the symmetry (1.9) is not needed at all to prove the main results of this paper. We assume them only to identify the gap equation analyzed here as that rigorously derived from the many-electron system based on these conditions in [13]. Crystalline lattices well studied in condensed matter physics can be expressed as $\mathcal{B}\times\Gamma$. For example $d=2$, $b=2$, $\mathbf{v}_1 = (1,0)^T$, $\mathbf{v}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})^T$ for the honeycomb lattice, $d=2$, $b=3$, $\mathbf{v}_1=(1,0)^T$, $\mathbf{v}_2=(0,1)^T$ for the Copper Oxide lattice. By tuning the onsite energy free Hamiltonians of hopping electron on these lattices can be formulated in the form (1.7) with some $E\in\mathcal{E}(e_{min}, e_{max})$. The Su-Schrieffer-Heeger (SSH) model ([22], [10]) and the Haldane model ([5], [8]) are benchmark models showing DQPTs at positive temperature. These models are originally spinless. Our free Hamiltonian covers their trivial extensions with spin. See [14, Remark 1.2] for formulating the SSH model and the Haldane model into the form (1.7).

In the infinite-volume limit $L\to\infty$ the momentum lattice Γ^* becomes the following set.

$$\Gamma^*_\infty := \left\{ \sum_{j=1}^d k_j\hat{\mathbf{v}}_j \;\middle|\; k_j\in[0,2\pi]\ (j=1,\cdots,d) \right\}\ (\subset\mathbb{R}^d).$$

For $E\in\mathcal{E}(e_{min}, e_{max})$ we define the function $g_E : \mathbb{R}_{>0}\times\mathbb{R}\times\mathbb{R}\to\mathbb{R}$ by

(1.12)

$g_E(x,t,z)$

$$:= -\frac{2}{|U|} + D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{\sinh(x\sqrt{E(\mathbf{k})^2+z^2})}{(\cos(t/2)+\cosh(x\sqrt{E(\mathbf{k})^2+z^2}))\sqrt{E(\mathbf{k})^2+z^2}} \right),$$

where $D_d := |\det(\hat{\mathbf{v}}_1, \cdots, \hat{\mathbf{v}}_d)|^{-1}(2\pi)^{-d}$ and $U \in \mathbb{R}_{<0}$. Originally the parameter U controls the strength of attractive interaction between Cooper pairs. For any function $f : \mathbb{R}\backslash\{0\} \to \mathbb{C}$ and non-singular Hermitian matrix $E \in \mathrm{Mat}(b, \mathbb{C})$ we define $f(E) \in \mathrm{Mat}(b, \mathbb{C})$ by the spectral decomposition. For $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$ we call the equation $g_E(\beta, t, \Delta) = 0$ with unknown $\Delta \in \mathbb{R}_{\ge 0}$ gap equation.

The free energy density derived in [13, Theorem 1.3 (ii)] explicitly depends on the gap function Δ. Let us recall the statement. For any proposition P $1_P := 1$ if P is true, $1_P := 0$ otherwise. Let $E \in \mathcal{E}(e_{min}, e_{max})$. For $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$ let $\Delta \in \mathbb{R}_{\ge 0}$ be a solution to the gap equation if exists. As we will see in Lemma 1.1, such Δ is unique. Set $\Delta := 0$ if there is no solution to the gap equation. If

$$U \in \left(-\frac{2c'}{b} \min\{e_{min}, e_{min}^{d+1}\}, 0 \right) \tag{1.13}$$

with $c' \in (0, 1]$ depending only on d, b, $(\hat{\mathbf{v}}_j)_{j=1}^d$ and the quantity

$$\sup_{\mathbf{k}\in\mathbb{R}^d} \sup_{\substack{m_j\in\mathbb{N}\cup\{0\} \\ (j=1,\cdots,d)}} \left\| \prod_{j=1}^d \frac{\partial^{m_j}}{\partial k_j^{m_j}} E(\mathbf{k}) \right\|_{b\times b} 1_{\sum_{j=1}^d m_j \le d+2},$$

$$\begin{aligned} &\lim_{\substack{L\to\infty \\ L\in\mathbb{N}}} \left(-\frac{1}{\beta L^d} \log(\mathrm{Tr}\, e^{-\beta \mathsf{H} + it\mathsf{S}_z}) \right) \\ &= \frac{\Delta^2}{|U|} - \frac{D_d}{\beta} \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr} \log \Bigg(2\cos\left(\frac{t}{2}\right) e^{-\beta E(\mathbf{k})} \\ &\qquad + e^{\beta(\sqrt{E(\mathbf{k})^2+\Delta^2} - E(\mathbf{k}))} + e^{-\beta(\sqrt{E(\mathbf{k})^2+\Delta^2} + E(\mathbf{k}))} \Bigg), \end{aligned} \tag{1.14}$$

where

$$\begin{aligned} &\mathsf{H} := \mathsf{H}_0 + \mathsf{V}, \\ &\mathsf{V} := \frac{U}{L^d} \sum_{\substack{(\rho,\mathbf{x}),(\eta,\mathbf{y}) \\ \in\mathcal{B}\times\Gamma}} \psi^*_{\rho\mathbf{x}\uparrow}\psi^*_{\rho\mathbf{x}\downarrow}\psi_{\eta\mathbf{y}\downarrow}\psi_{\eta\mathbf{y}\uparrow},\ \mathsf{S}_z := \frac{1}{2} \sum_{(\rho,\mathbf{x})\in\mathcal{B}\times\Gamma} (\psi^*_{\rho\mathbf{x}\uparrow}\psi_{\rho\mathbf{x}\uparrow} - \psi^*_{\rho\mathbf{x}\downarrow}\psi_{\rho\mathbf{x}\downarrow}). \end{aligned} \tag{1.15}$$

The operator V is the reduced BCS interaction and S_z is the z-component of the spin operator. The operator H is called the BCS model or the reduced BCS model because of the form of interaction. For clarity we remark that in [13, Theorem 1.3 (ii)] the infinite-volume limit

$$\lim_{\substack{L\to\infty \\ L\in\mathbb{N}}} \left(-\frac{1}{\beta L^d} \log(\mathrm{Tr}\, e^{-\beta(\mathsf{H} + i\theta\mathsf{S}_z)}) \right)$$

with $\theta \in \mathbb{R}$ was derived. Since the real parameter θ can be chosen arbitrarily, the above statement follows. The Fermionic operators appear only in this subsection.

As summarized in Lemma 1.3 later, the free energy density loses analyticity on the boundary of the domain of (β, t) where the gap equation has a positive solution.

To describe this precisely, we need to know properties of the gap equation. The following lemma is essentially the same as [13, Lemma 1.2]. However, as it is important for the present paper, let us give the proof here. The claim (iv) provides the rigorous version of (1.6). Let $\tanh^{-1} : (-1,1) \to \mathbb{R}$ be the inverse function of $\tanh : \mathbb{R} \to (-1,1)$.

Lemma 1.1. *Assume that $U \in (-\frac{2e_{min}}{b}, 0)$. Then there uniquely exists*

$$\beta_c \in \left(0, \frac{2}{e_{min}} \tanh^{-1}\left(\frac{b|U|}{2e_{min}}\right)\right]$$

such that the following statements hold.

(i) If $\beta > \beta_c$, $g_E(\beta,t,z) \neq 0$ for any $(t,z) \in \mathbb{R} \times \mathbb{R}_{\geq 0}$.

(ii) $g_E(\beta_c,t,\Delta) = 0$ with $(t,\Delta) \in \mathbb{R} \times \mathbb{R}_{\geq 0}$ if and only if $t = 2\pi$ (mod 4π) and $\Delta = 0$.

(iii) If $0 < \beta < \beta_c$, there exists $(t,\Delta) \in \mathbb{R} \times \mathbb{R}_{>0}$ such that $g_E(\beta,t,\Delta) = 0$. Such Δ is unique. Moreover there uniquely exists $\tau(\beta) \in (\pi, 2\pi)$ such that $g_E(\beta, \delta\tau(\beta) + 4m\pi, 0) = 0$ for any $\delta \in \{-1,1\}$, $m \in \mathbb{Z}$.

(iv) Let the function $\beta \mapsto \tau(\beta) : (0,\beta_c) \to (\pi, 2\pi)$ be defined by the claim (iii).

(1.16)

$$\begin{aligned}
&\{(\beta,t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \text{there uniquely exists } \Delta \in \mathbb{R}_{>0} \text{ such that } g_E(\beta,t,\Delta) = 0\} \\
&= \{(\beta,t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid g_E(\beta,t,0) > 0\} \\
&= \bigsqcup_{m\in\mathbb{Z}} \{(\beta,t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \beta \in (0,\beta_c),\ t \in (\tau(\beta) + 4m\pi, -\tau(\beta) + 4(m+1)\pi)\}.
\end{aligned}$$

Proof. Observe that

$$g_E(\beta, 2\pi, 0) = -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta}{2}E(\mathbf{k}))E(\mathbf{k})}\right).$$

It follows that $\beta \mapsto g_E(\beta, 2\pi, 0)$ is strictly monotone decreasing and

$$\lim_{\beta \searrow 0} g_E(\beta, 2\pi, 0) = +\infty, \ \lim_{\beta \nearrow \infty} g_E(\beta, 2\pi, 0) \leq -\frac{2}{|U|} + \frac{b}{e_{min}} < 0.$$

Thus there uniquely exists $\beta_c \in \mathbb{R}_{>0}$ such that $g_E(\beta_c, 2\pi, 0) = 0$. Moreover

$$0 \leq -\frac{2}{|U|} + \frac{b}{\tanh(\frac{\beta_c}{2}e_{min})e_{min}}$$

or

$$\beta_c \leq \frac{2}{e_{min}} \tanh^{-1}\left(\frac{b|U|}{2e_{min}}\right).$$

The following property is useful.

(1.17) For any $(\beta,t) \in \mathbb{R}_{>0} \times \mathbb{R}$, $z \mapsto g_E(\beta,t,z) : \mathbb{R}_{\geq 0} \to \mathbb{R}$ is strictly monotone decreasing. Moreover, $\lim_{z\to\infty} g_E(\beta,t,z) = -\frac{2}{|U|} < 0.$

The claimed decreasing property can be confirmed by showing that

$$\frac{d}{dX}\left(\frac{1}{a+\cosh(X)}\right)\cdot\frac{\sinh(X)}{X} + \frac{1}{a+\cosh(X)}\frac{d}{dX}\left(\frac{\sinh(X)}{X}\right) < 0,$$
$$\forall a \in [-1,1],\ X \in \mathbb{R}_{>0}.$$

By (1.17)

$$g_E(\beta,t,z) \le g_E(\beta,t,0) \le g_E(\beta,2\pi,0) < g_E(\beta_c,2\pi,0) = 0,$$
$$\forall(\beta,t,z) \in (\beta_c,\infty)\times\mathbb{R}\times\mathbb{R}_{\ge 0}.$$

Thus the claim (i) holds.

If $t \ne 2\pi \pmod{4\pi}$, $\Delta \in \mathbb{R}_{\ge 0}$ and $g_E(\beta_c,t,\Delta) = 0$,

$$0 = g_E(\beta_c,t,\Delta) < g_E(\beta_c,2\pi,\Delta) \le g_E(\beta_c,2\pi,0) = 0,$$

which is a contradiction. If $t \in \mathbb{R}$, $\Delta > 0$ and $g_E(\beta_c,t,\Delta) = 0$,

$$0 = g_E(\beta_c,t,\Delta) < g_E(\beta_c,t,0) \le g_E(\beta_c,2\pi,0) = 0,$$

which is again a contradiction. Thus, if $g_E(\beta_c,t,\Delta) = 0$ with $(t,\Delta) \in \mathbb{R}\times\mathbb{R}_{\ge 0}$, $t = 2\pi \pmod{4\pi}$ and $\Delta = 0$. The converse is clear. The claim (ii) holds.

If $\beta \in (0,\beta_c)$,

$$g_E(\beta,2\pi,0) > g_E(\beta_c,2\pi,0) = 0, \quad \lim_{z\to\infty} g_E(\beta,2\pi,z) = -\frac{2}{|U|} < 0.$$

These imply that there exists $(t,\Delta) \in \mathbb{R}\times\mathbb{R}_{>0}$ such that $g_E(\beta,t,\Delta) = 0$. By (1.17) such Δ is unique. By assumption $g_E(\beta,\pi,0) \le -\frac{2}{|U|} + \frac{b}{e_{min}} < 0$. Since $g_E(\beta,2\pi,0) > 0$, there uniquely exists $\tau(\beta) \in (\pi,2\pi)$ such that $g_E(\beta,\delta\tau(\beta)+4m\pi,0) = 0$ for any $\delta \in \{-1,1\}$, $m \in \mathbb{Z}$. This ensures the claim (iii).

One can deduce the first equality of (1.16) from the property (1.17). For any $\beta \in (0,\beta_c)$, $m \in \mathbb{Z}$, $t \in (\tau(\beta)+4m\pi, -\tau(\beta)+4(m+1)\pi)$ $g_E(\beta,t,0) > g_E(\beta,\tau(\beta),0) = 0$. Conversely let us assume that $(\beta,t) \in \mathbb{R}_{>0}\times\mathbb{R}$ and $g_E(\beta,t,0) > 0$. By (1.17) there exists $\Delta \in \mathbb{R}_{>0}$ such that $g_E(\beta,t,\Delta) = 0$. By (i), (ii) $\beta < \beta_c$. If $t \notin (\tau(\beta)+4m\pi, -\tau(\beta)+4(m+1)\pi)$ for any $m \in \mathbb{Z}$, $g_E(\beta,t,0) \le g_E(\beta,\tau(\beta),0) = 0$. Contradiction. Thus there exists $m \in \mathbb{Z}$ such that $t \in (\tau(\beta)+4m\pi, -\tau(\beta)+4(m+1)\pi)$. The second equality of (1.16) is also proved. □

In order to ensure the existence of the critical inverse temperature β_c, we always deal with $U \in \mathbb{R}_{<0}$ satisfying $|U| < \frac{2e_{min}}{b}$ in this paper. The negative parameter U controls the strength of attractive interaction. See (1.15). The sign of U matters in the derivation of the gap equation from the many-electron system. In this paper, however, the sign plays no essential role.

Concerning the function $\tau : (0,\beta_c) \to (\pi,2\pi)$, more detailed properties are known.

Lemma 1.2. *([13, Lemma 2.2])*

(i) τ *is real analytic in* $(0, \beta_c)$.

(ii)

$$\lim_{\beta \nearrow \beta_c} \tau(\beta) = \lim_{\beta \searrow 0} \tau(\beta) = 2\pi.$$

(iii)

$$\lim_{\beta \nearrow \beta_c} \frac{d\tau}{d\beta}(\beta) = +\infty, \ \lim_{\beta \searrow 0} \frac{d\tau}{d\beta}(\beta) = -\infty.$$

To state the rigorous version of the relation (1.5), we define the function $\Delta : \mathbb{R}_{>0} \times \mathbb{R} \to \mathbb{R}_{\geq 0}$ as follows. For $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$, if $g_E(\beta, t, 0) > 0$, $\Delta(\beta, t)(\in \mathbb{R}_{>0})$ is the unique solution to the gap equation. Otherwise $\Delta(\beta, t) := 0$. By (1.16) the function Δ is well-defined. Then we define the function $(\beta, t) \mapsto F_E(\beta, t) : \mathbb{R}_{>0} \times \mathbb{R} \to \mathbb{R}$ by the right-hand side of (1.14) with $\Delta = \Delta(\beta, t)$. In fact we do not use the following lemma to prove the main results of this paper. We state it only to understand the meaning of the sets analyzed as the main objects in this paper.

Lemma 1.3. *Assume that* $U \in (-\frac{2e_{min}}{b}, 0)$. *Then the following equalities hold.*

$$\begin{aligned}
&\{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \textit{the function } F_E \textit{ is not analytic at } (\beta, t)\} \\
&= \{(\beta, t_0) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \textit{the function } t \mapsto F_E(\beta, t) \textit{ is not analytic at } t = t_0\} \\
&\quad \cup \{(\beta_c, 2\pi + 4\pi m) \mid m \in \mathbb{Z}\} \\
&= \bigsqcup_{m \in \mathbb{Z}} \{(\beta, \tau(\beta) + 4m\pi), \ (\beta, -\tau(\beta) + 4(m+1)\pi) \mid \beta \in (0, \beta_c)\} \cup \{(\beta_c, 2\pi + 4\pi m)\} \\
&= \partial\{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \Delta(\beta, t) > 0\} \cap \mathbb{R}_{>0} \times \mathbb{R}.
\end{aligned}$$

For any subset S *of* $\mathbb{R}^2$ ∂S *denotes its boundary in* $\mathbb{R}^2$.

Proof. The 1st and the 2nd equality follows from [13, (2.3), Proposition 2.5]. The 3rd equality follows from (1.16) and Lemma 1.2. □

Remark 1.4. Since $\Delta(\beta_c, t) = 0$ for any $t \in \mathbb{R}$, $t \mapsto F_E(\beta_c, t)$ is analytic in $\mathbb{R}$. This together with Lemma 1.3 implies that

$$\begin{aligned}
&\{(\beta, t_0) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \text{the function } t \mapsto F_E(\beta, t) \text{ is not analytic at } t = t_0\} \\
&= \bigsqcup_{m \in \mathbb{Z}} \{(\beta, \tau(\beta) + 4m\pi), \ (\beta, -\tau(\beta) + 4(m+1)\pi) \mid \beta \in (0, \beta_c)\}.
\end{aligned}$$

Since DQPT is defined by non-analyticity of $F_E(\beta, t)$ with the real time variable t, the above equality characterizes the phase boundary of DQPT in the BCS model.

The above lemma suggests that the phase boundary is the disjoint union of periodic copies of the representative simple curve

$$C_0 = \{(\beta, \tau(\beta)), \ (\beta, -\tau(\beta) + 4\pi) \mid \beta \in (0, \beta_c)\} \cup \{(\beta_c, 2\pi)\}.$$

To analyze the whole phase boundary, it suffices to focus on the function $\tau : (0, \beta_c) \to (\pi, 2\pi)$. Moreover, Lemma 1.1 (iv) suggests that the domain of (β, t) where the gap equation has a positive solution consists of periodic copies of the representative set S_0 defined by

$$S_0 := \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \beta \in (0, \beta_c), \ t \in (\tau(\beta), -\tau(\beta) + 4\pi)\}.$$

Observe that $C_0 = \partial S_0 \cap \mathbb{R}_{>0} \times \mathbb{R}$. The set S_0 is pictured in Figure 1.

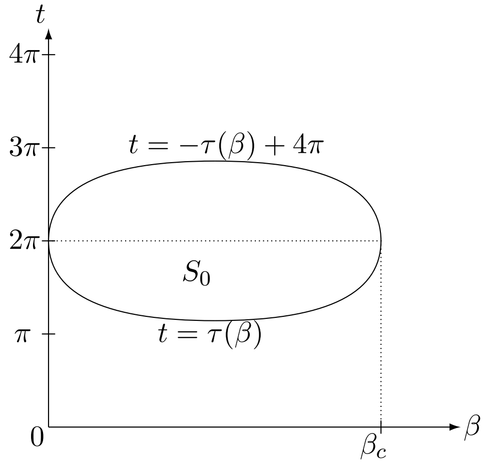

Figure 1: The representative set S_0 and its boundary.

Remark 1.5. In [13, Proposition 2.4] we proved that $C_0 \cup \{(0, 2\pi)\}$ is a 1-dimensional real analytic submanifold of $\mathbb{R}^2$.

The main results of this paper concern convexity of the function $\tau(\cdot)$ and the set S_0. Specifically Proposition 1.6, Proposition 1.7, Proposition 1.8 and Theorem 1.11 are the main results.

Proposition 1.6. *Assume that* $\frac{e_{min}}{e_{max}} > \sqrt{9 - 4\sqrt{5}}$. *Then there exists* $U_0 \in (0, \frac{e_{min}}{\sinh(2)b}]$ *such that for any* $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$ *and* $\beta \in (0, \beta_c)$ $\frac{d^2\tau}{d\beta^2}(\beta) > 0$. *Moreover*

$$\lim_{\beta \nearrow \beta_c} \frac{d^2\tau}{d\beta^2}(\beta) = +\infty, \ \lim_{\beta \searrow 0} \frac{d^2\tau}{d\beta^2}(\beta) = +\infty.$$

The convexity of $\tau(\cdot)$ does not always hold when $\frac{e_{min}}{e_{max}} \leq \sqrt{9 - 4\sqrt{5}}$.

Proposition 1.7. *Assume that* $\frac{e_{min}}{e_{max}} < \sqrt{9 - 4\sqrt{5}}$. *Then there exist* $U_0 \in (0, \frac{2e_{min}}{b})$, $E \in \mathcal{E}(e_{min}, e_{max})$ *such that the following statement holds. For any* $U \in [-U_0, 0)$ *there exists* $\beta \in (0, \beta_c)$ *such that* $\frac{d^2\tau}{d\beta^2}(\beta) < 0$.

When $\frac{e_{min}}{e_{max}} = \sqrt{9 - 4\sqrt{5}}$, a slightly weaker conclusion holds. More precisely, the choice of E depends on U.

Proposition 1.8. *Assume that* $\frac{e_{min}}{e_{max}} = \sqrt{9 - 4\sqrt{5}}$. *Then there exists* $U_0 \in (0, \frac{2e_{min}}{b})$ *such that the following statement holds. For any* $U \in [-U_0, 0)$ *there exist* $E \in \mathcal{E}(e_{min}, e_{max})$, $\beta \in (0, \beta_c)$ *such that* $\frac{d^2\tau}{d\beta^2}(\beta) < 0$.

Remark 1.9. We should remark at this stage that the proof of Proposition 1.8 relies on exact calculations of low order terms of power series expansion of an analytic function, which is the most complicated part in this paper. On the other hand, Proposition 1.6, Proposition 1.7 can be proven more systematically.

We combine these propositions to characterize the convexity of the set S_0 as the main theorem. Let us confirm basic relations between the 2nd order derivative of $\tau(\cdot)$ and the convexity of S_0. Remind us that for any set $S \subset \mathbb{R}^n$ S is called convex if $s\mathbf{x}_1 + (1-s)\mathbf{x}_2 \in S$ for any $\mathbf{x}_1, \mathbf{x}_2 \in S$, $s \in [0, 1]$.

Lemma 1.10. *(i) If $\frac{d^2\tau}{d\beta^2}(\beta) > 0$ for any $\beta \in (0, \beta_c)$, S_0 is convex.*

(ii) If there exists $\beta \in (0, \beta_c)$ such that $\frac{d^2\tau}{d\beta^2}(\beta) < 0$, S_0 is not convex.

Proof. (i): Take any (β_1, t_1), $(\beta_2, t_2) \in S_0$ and $s \in [0, 1]$. By the assumption

$$\begin{aligned}&\tau(s\beta_1 + (1-s)\beta_2) \le s\tau(\beta_1) + (1-s)\tau(\beta_2) < st_1 + (1-s)t_2,\\ &4\pi - \tau(s\beta_1 + (1-s)\beta_2) \ge s(4\pi - \tau(\beta_1)) + (1-s)(4\pi - \tau(\beta_2)) > st_1 + (1-s)t_2.\end{aligned}$$

Thus $s(\beta_1, t_1) + (1-s)(\beta_2, t_2) \in S_0$. Therefore S_0 is convex.

(ii): By the assumption there exist β_1, $\beta_2 \in (0, \beta_c)$, $s \in (0, 1)$ such that $\tau(s\beta_1 + (1-s)\beta_2) > s\tau(\beta_1) + (1-s)\tau(\beta_2)$. We can choose small $\varepsilon > 0$ so that

$$\begin{aligned}&\tau(\beta_j) + \varepsilon < 2\pi \ (j = 1, 2),\\ &\tau(s\beta_1 + (1-s)\beta_2) > s(\tau(\beta_1) + \varepsilon) + (1-s)(\tau(\beta_2) + \varepsilon).\end{aligned}$$

Thus $(\beta_j, \tau(\beta_j) + \varepsilon) \in S_0$ $(j = 1, 2)$ and

$$s(\beta_1, \tau(\beta_1) + \varepsilon) + (1-s)(\beta_2, \tau(\beta_2) + \varepsilon) \notin S_0.$$

Therefore S_0 is not convex. $\square$

By combining Proposition 1.6, Proposition 1.7, Proposition 1.8 and Lemma 1.10 we can deduce the following theorem.

Theorem 1.11. *For any $d, b \in \mathbb{N}$, basis $(\hat{\mathbf{v}}_j)_{j=1}^d$ of $\mathbb{R}^d$ and e_{min}, $e_{max} \in \mathbb{R}_{>0}$ satisfying $e_{min} \le e_{max}$ the following statements are equivalent to each other.*

(i) There exists $U_0 \in (0, \frac{2e_{min}}{b})$ such that for any $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$ and $\beta \in (0, \beta_c)$ $\frac{d^2\tau}{d\beta^2}(\beta) > 0$.

(ii) There exists $U_0 \in (0, \frac{2e_{min}}{b})$ such that for any $U \in [-U_0, 0)$ and $E \in \mathcal{E}(e_{min}, e_{max})$ S_0 is convex.

(iii) $\frac{e_{min}}{e_{max}} > \sqrt{9 - 4\sqrt{5}}$.

Proof. The equivalence between (i) and (iii) follows from Proposition 1.6, Proposition 1.7 and Proposition 1.8. By Lemma 1.10 (i) the claim (i) implies the claim (ii). If (iii) does not hold, by Proposition 1.7 and Proposition 1.8 for any $U_0 \in (0, \frac{2e_{min}}{b})$ there exist $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$ and $\beta \in (0, \beta_c)$ such that $\frac{d^2\tau}{d\beta^2}(\beta) < 0$. Thus by Lemma 1.10 (ii) S_0 is not convex, which means that (ii) does not hold. Therefore (ii) implies (iii). The claims (i), (ii), (iii) are equivalent to each other. $\square$

Remark 1.12. The behavior of $\frac{d^2\tau}{d\beta^2}(\cdot)$ claimed in Proposition 1.6, Proposition 1.7 and Proposition 1.8 implies a physical property of the phase transition, which is so-called reentrant phenomenon along a line drawn in the phase diagram. Mathematically we define the reentry into the exterior from the interior as follows. Take $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}_{>0} \times \mathbb{R}$ satisfying $\mathbf{x}_1 \ne \mathbf{x}_2$.

(EIE)$(\mathbf{x}_1, \mathbf{x}_2)$ There exists $\varepsilon \in \mathbb{R}_{>0}$ such that

$$\begin{aligned}&\Delta(s\mathbf{x}_1 + (1-s)\mathbf{x}_2) > 0, \ \forall s \in (0, 1),\\ &\Delta(s\mathbf{x}_1 + (1-s)\mathbf{x}_2) = 0, \ \forall s \in [-\varepsilon, 0] \cup [1, 1+\varepsilon].\end{aligned}$$

Similarly we define the reentry into the interior from the exterior as below.

(IEI)$(\mathbf{x}_1,\mathbf{x}_2)$ There exists $\varepsilon\in\mathbb{R}_{>0}$ such that
$\Delta(s\mathbf{x}_1+(1-s)\mathbf{x}_2)=0,\ \forall s\in[0,1]$,
$\Delta(s\mathbf{x}_1+(1-s)\mathbf{x}_2)>0,\ \forall s\in[-\varepsilon,0)\cup(1,1+\varepsilon]$.

Recalling the definition of the simple curve C_0, we can confirm the following.

- If $\frac{d^2\tau}{d\beta^2}(\beta)>0$ for any $\beta\in(0,\beta_c)$, then for any $\mathbf{x}_1,\mathbf{x}_2\in C_0$ with $\mathbf{x}_1\neq\mathbf{x}_2$ (EIE)$(\mathbf{x}_1,\mathbf{x}_2)$ holds.
- If $\frac{d^2\tau}{d\beta^2}(\beta)<0$ for some $\beta\in(0,\beta_c)$, then for any $\delta\in\mathbb{R}_{>0}$ there exist $\mathbf{x}_1,\mathbf{x}_2\in C_0$ such that $0<\|\mathbf{x}_1-\mathbf{x}_2\|_{\mathbb{R}^2}<\delta$ and (IEI)$(\mathbf{x}_1,\mathbf{x}_2)$ holds.

Accordingly we can replace the conclusion "for any $\beta\in(0,\beta_c)$ $\frac{d^2\tau}{d\beta^2}(\beta)>0$" by "for any $\mathbf{x}_1,\mathbf{x}_2\in C_0$ with $\mathbf{x}_1\neq\mathbf{x}_2$ (EIE)$(\mathbf{x}_1,\mathbf{x}_2)$ holds." in the statement of Proposition 1.6. Also we can replace the conclusion "there exists $\beta\in(0,\beta_c)$ such that $\frac{d^2\tau}{d\beta^2}(\beta)<0$" by "for any $\delta\in\mathbb{R}_{>0}$ there exists $\mathbf{x}_1,\mathbf{x}_2\in C_0$ such that $0<\|\mathbf{x}_1-\mathbf{x}_2\|_{\mathbb{R}^2}<\delta$ and (IEI)$(\mathbf{x}_1,\mathbf{x}_2)$ holds." in the statements of Proposition 1.7, Proposition 1.8.

Remark 1.13. We are analyzing the phase boundary where the function F_E loses analyticity. However, it is not obvious if we can prove the derivation of F_E from the many-electron system as stated in (1.14) together with the main results of this paper. By considering the fact that $c'\in(0,1]$ depends on the derivatives of E we can deduce the following from Proposition 1.6 and Proposition 1.7.

- If $\frac{e_{min}}{e_{max}}>\sqrt{9-4\sqrt{5}}$, for any $E\in\mathcal{E}(e_{min},e_{max})$ there exists $U_0\in(0,\frac{e_{min}}{\sinh(2)b}]$ such that for any $U\in[-U_0,0)$, $\beta\in(0,\beta_c)$ $\frac{d^2\tau}{d\beta^2}(\beta)>0$ and the equality (1.14) is justified.
- If $\frac{e_{min}}{e_{max}}<\sqrt{9-4\sqrt{5}}$, there exist $U_0\in(0,\frac{2e_{min}}{b})$, $E\in\mathcal{E}(e_{min},e_{max})$ such that for any $U\in[-U_0,0)$ $\frac{d^2\tau}{d\beta^2}(\beta)<0$ for some $\beta\in(0,\beta_c)$ and the equality (1.14) is justified.

As we will see in Section 4, we have to choose $E\in\mathcal{E}(e_{min},e_{max})$ after fixing $U\in[-U_0,0)$ in the proof of Proposition 1.8. It is not clear if the condition (1.13) is satisfied in this situation. Therefore we cannot prove non-convexity of the phase boundary in case that $\frac{e_{min}}{e_{max}}=\sqrt{9-4\sqrt{5}}$ as claimed in Proposition 1.8 while justifying the equality (1.14).

Remark 1.14. In the preceding papers [13], [14] we had numerical examples showing non-convexity of the function $\tau:(0,\beta_c)\to\mathbb{R}$. The picture [13, Figure 2, (b)] shows the graph of $\tau(\cdot)$ having 2 local mininum points when $\frac{e_{min}}{e_{max}}=\frac{1}{7}(<\sqrt{9-4\sqrt{5}})$. The pictures in [14, Figure 4] show that $\frac{d\tau}{d\beta}(\cdot)$ can be decreasing when $\frac{e_{min}}{e_{max}}=\frac{1}{8.342},\frac{1}{6.643}(<\sqrt{9-4\sqrt{5}})$.

Remark 1.15. Here we can summarize the main results of [13, Section 2], [14] and this paper concerning the behavior of $\tau(\cdot)$ more rigorously than in Subsection 1.1. Let P be a proposition and c_r be a positive constant. We have been proving the following statement.

For any $d,b\in\mathbb{N}$, basis $(\hat{\mathbf{v}}_j)_{j=1}^d$ of $\mathbb{R}^d$ and $e_{min},e_{max}\in\mathbb{R}_{>0}$ satisfying $e_{min}\le e_{max}$ (i), (ii) are equivalent to each other.

(i) There exists $U_0 \in (0, \frac{2e_{min}}{b})$ such that for any $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$ P holds.

(ii) $\frac{e_{min}}{e_{max}} > c_r$.

The proposition P and the constant c_r are given as below.

- In [13, Theorem 2.19]

$$P: \ \tau(\cdot) \text{ has only one local minimum point in } (0, \beta_c).$$
$$c_r = \sqrt{17 - 12\sqrt{2}}.$$

- In [14, Theorem 1.8]

$$P: \ \tau(\cdot) \text{ has no stationary point of inflection in } (0, \beta_c).$$
$$c_r = \sqrt{17 - 12\sqrt{2}}.$$

- In Theorem 1.11 of this paper

$$P: \ \frac{d^2\tau}{d\beta^2}(\beta) > 0 \text{ for any } \beta \in (0, \beta_c).$$
$$c_r = \sqrt{9 - 4\sqrt{5}}.$$

Remark 1.16. In [13, Proposition 2.8] we proved that if $\frac{e_{min}}{e_{max}} \geq e_0$ for some $e_0 \in (0, 1)$, $\frac{d^2\tau}{d\beta^2}(\beta) > 0$ for any $U \in [-\frac{e_{min}}{\sinh(2)b}, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$ and $\beta \in (0, \beta_c)$. Since the proof was based on non-optimal estimations, we were unable to find the optimal value of such e_0 there. Theorem 1.11 here presents an optimal value $\sqrt{9 - 4\sqrt{5}}$.

Remark 1.17. Some may be more accustomed to a graph with temperature than inverse temperature. Here let us remark what we know on the behavior of the function $T \mapsto \tau(\frac{1}{T}) : (\frac{1}{\beta_c}, \infty) \to (\pi, 2\pi)$. Based on the equality $\frac{d}{dT}(\tau(\frac{1}{T})) = -\frac{1}{T^2}\frac{d\tau}{d\beta}(\frac{1}{T})$ and [13, Theorem 2.19], [14, Theorem 1.8], we can characterize uniqueness of a local minimum point and non-existence of a stationary point of inflection by the constant $\sqrt{17 - 12\sqrt{2}}$ in the same way as in Remark 1.15. Regardless of the value of $\frac{e_{min}}{e_{max}}$, the function $T \mapsto \tau(\frac{1}{T})$ is not convex, i.e. $\frac{d^2}{dT^2}(\tau(\frac{1}{T})) < 0$ for some $T \in (\frac{1}{\beta_c}, \infty)$. This can be deduced from the properties that $\tau(\frac{1}{T}) < 2\pi$ for any $T \in (\frac{1}{\beta_c}, \infty)$ and $\lim_{T \to \infty} \tau(\frac{1}{T}) = 2\pi$.

Remark 1.18. One basic assumption in this paper is the weak coupling condition $|U| < \frac{2e_{min}}{b}$. There are two reasons why we always assume this. Firstly, the condition (1.13) under which the free energy density together with the gap equation is rigorously derived in [13, Theorem 1.3] implies this inequality, and thus we can interpret the main results Proposition 1.6, Proposition 1.7 as rigorous properties of the infinite-volume limit of the microscopic model by assuming (1.13) from the beginning. This is explained in Remark 1.13 in more detail. Secondly, under this condition the phase boundary has universal properties as described in Lemma 1.1, Lemma 1.2 and Lemma 1.3. We have decided to focus on the analysis of these properties. It is possible to define the gap equation alone under the strong coupling condition $|U| \geq \frac{2e_{min}}{b}$, though the derivation from the microscopic model cannot be proved by the multi-scale analysis we have developed in this series. Under the condition $|U| \geq \frac{2e_{min}}{b}$ the phase boundary can radically change its geometric properties, depending on the choice of $E \in \mathcal{E}(e_{min}, e_{max})$. Here let us summarize some of the basic provable properties by putting the issue of derivation aside.

For $E \in \mathcal{E}(e_{min}, e_{max})$, set

$$g_E^{\infty} := -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{|E(\mathbf{k})|}\right).$$

Observe that $g_E^{\infty} = \lim_{\beta \nearrow \infty} g_E(\beta, t, 0)$ for any $t \in \mathbb{R}$. While $g_E^{\infty} < 0$ for any $E \in \mathcal{E}(e_{min}, e_{max})$ if $|U| < \frac{2e_{min}}{b}$, g_E^{∞} can change its sign, depending on the choice of $E \in \mathcal{E}(e_{min}, e_{max})$, if $|U| \geq \frac{2e_{min}}{b}$. There are three cases.

(Case 1) $\quad g_E^{\infty} < 0.$

(Case 2) $\quad g_E^{\infty} = 0.$

(Case 3) $\quad g_E^{\infty} > 0.$

For example if $|U| = \frac{2e_{min}}{b}$, $0 < b' < b$, $0 < e_{min} < e_{max}$ and

$$E = \begin{pmatrix} e_{min} I_{b'} & 0 \\ 0 & e_{max} I_{b-b'} \end{pmatrix},$$

(Case 1) holds. If $|U| = \frac{2e_{min}}{b}$, $e_{min} = e_{max}$ and $E = e_{min} I_b$, (Case 2) holds. If $|U| > \frac{2e_{min}}{b}$, $e_{min} = e_{max}$ and $E = e_{min} I_b$, (Case 3) holds. Here let us characterize the set

$$D_> = \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \text{there uniquely exists } \Delta \in \mathbb{R}_{>0} \text{ such that } g_E(\beta, t, \Delta) = 0\}$$

in a manner similar to Lemma 1.1 (iv).

- In (Case 1) there exists $\beta_c \in \mathbb{R}_{>0}$ and $\tau : (0, \beta_c) \to (\pi, 2\pi)$ such that $\lim_{\beta \searrow 0} \tau(\beta) = 2\pi$, $\lim_{\beta \nearrow \beta_c} \tau(\beta) = 2\pi$,

$$D_> = \bigsqcup_{m \in \mathbb{Z}} \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \beta \in (0, \beta_c),\ t \in (\tau(\beta) + 4m\pi, -\tau(\beta) + 4(m+1)\pi)\}.$$

- In (Case 2) there exists $\tau : \mathbb{R}_{>0} \to (\pi, 2\pi)$ such that $\lim_{\beta \searrow 0} \tau(\beta) = 2\pi$,

$$D_> = \bigsqcup_{m \in \mathbb{Z}} \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid t \in (\tau(\beta) + 4m\pi, -\tau(\beta) + 4(m+1)\pi)\}.$$

- In (Case 3) there exists $\beta_c \in \mathbb{R}_{>0}$ and $\tau : (0, \beta_c) \to (0, 2\pi)$ such that $\lim_{\beta \searrow 0} \tau(\beta) = 2\pi$, $\lim_{\beta \nearrow \beta_c} \tau(\beta) = 0$,

$$D_> = \bigsqcup_{m \in \mathbb{Z}} \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid \beta \in (0, \beta_c),\ t \in (\tau(\beta) + 4m\pi, -\tau(\beta) + 4(m+1)\pi)\} \sqcup \{\beta_c\} \times \mathbb{R} \backslash 4\pi\mathbb{Z} \sqcup (\beta_c, \infty) \times \mathbb{R}.$$

In (Case 1) the situation is close to that under the condition $|U| < \frac{2e_{min}}{b}$. However in (Case 2) the phase boundary exists for all $\beta \in \mathbb{R}_{>0}$. Also in (Case 3) the gap function Δ is positive for any $(\beta, t) \in (\beta_c, \infty) \times \mathbb{R}$. So the phase diagram is globally different in these cases. Detailed analysis of them is open at present.

Remark 1.19. As we have already mentioned in Subsection 1.1, the characteristic function of the work done in our many-body system by changing the Hamiltonian H to $\mathsf{H} + \mathsf{S}_z$ is equal to (1.4). See [23] for the derivation. The work distribution function is its Fourier transform. We note that

$$\frac{\mathrm{Tr}(e^{-\beta\mathsf{H}}e^{-it\mathsf{H}}e^{it(\mathsf{H}+\mathsf{S}_z)})}{\mathrm{Tr}\, e^{-\beta\mathsf{H}}} = \sum_{n=-bL^d}^{bL^d} e^{it\frac{n}{2}} \frac{\mathrm{Tr}_n\, e^{-\beta\mathsf{H}}}{\mathrm{Tr}\, e^{-\beta\mathsf{H}}},$$

where $\mathrm{Tr}_n\, e^{-\beta\mathsf{H}}$ denotes the trace of $e^{-\beta\mathsf{H}}$ over the subspace

$$\left\{\psi \in F_f(L^2(\mathcal{B} \times \Gamma \times \{\uparrow, \downarrow\})) \;\middle|\; \mathsf{S}_z\psi = \frac{n}{2}\psi\right\}.$$

This implies that the possible values of the work are $\frac{n}{2}$ ($n = -bL^d, -bL^d+1, \cdots, bL^d$) and the work distribution function $P_L(\cdot)$ is given by

$$P_L(w) = \frac{1}{4\pi}\int_{-2\pi}^{2\pi} dt e^{-itw} \frac{\mathrm{Tr}(e^{-\beta\mathsf{H}}e^{-it\mathsf{H}}e^{it(\mathsf{H}+\mathsf{S}_z)})}{\mathrm{Tr}\, e^{-\beta\mathsf{H}}},$$
$$w \in \left\{\frac{n}{2} \;\middle|\; n = -bL^d, -bL^d + 1, \cdots, bL^d\right\}.$$

Observe that

$$P_L\left(\frac{n}{2}\right) = \frac{\mathrm{Tr}_n\, e^{-\beta\mathsf{H}}}{\mathrm{Tr}\, e^{-\beta\mathsf{H}}} \ge 0,\ \forall n \in \{-bL^d, -bL^d + 1, \cdots, bL^d\},$$
$$\sum_{n=-bL^d}^{bL^d} P_L\left(\frac{n}{2}\right) = 1. \tag{1.18}$$

Properties of work statistics after quantum quench have been studied in physics literature (e.g. [21], [9], [1]). For example the letter [21] demonstrates via analysis of Loschmidt echo that the work distribution function can diverge to infinity in case of a local quench in a quantum Ising chain. Here let us derive one property of our work distribution function from our previous results. Set

$$\mathcal{P}(\beta, L) := \sum_{n=-bL^d}^{bL^d} \left(1_{n \text{ is even}} P_L\left(\frac{n}{2}\right) - 1_{n \text{ is odd}} P_L\left(\frac{n}{2}\right)\right)$$

so that

$$\mathcal{P}(\beta, L) = \frac{\mathrm{Tr}\, e^{-\beta\mathsf{H}+i2\pi\mathsf{S}_z}}{\mathrm{Tr}\, e^{-\beta\mathsf{H}}}.$$

It follows from [13, Theorem 1.3, Proposition 2.5 (ii)] that if U satisfies the condition (1.13), $\mathcal{P}(\beta, L) > 0$ for sufficiently large $L \in \mathbb{N}$, $\lim_{L\to\infty, L\in\mathbb{N}} \frac{1}{L^d}\log\mathcal{P}(\beta, L)$ exists, $\beta \mapsto \lim_{L\to\infty, L\in\mathbb{N}} \frac{1}{L^d}\log\mathcal{P}(\beta, L)$ is C^1-class in $\mathbb{R}_{>0}$,

$$\lim_{\beta\nearrow\beta_c} \frac{\partial^2}{\partial\beta^2} \lim_{\substack{L\to\infty\\ L\in\mathbb{N}}} \frac{1}{L^d}\log\mathcal{P}(\beta, L),\ \lim_{\beta\searrow\beta_c} \frac{\partial^2}{\partial\beta^2} \lim_{\substack{L\to\infty\\ L\in\mathbb{N}}} \frac{1}{L^d}\log\mathcal{P}(\beta, L)$$

exist and

$$\lim_{\beta\nearrow\beta_c}\frac{\partial^2}{\partial\beta^2}\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}}\frac{1}{L^d}\log\mathcal{P}(\beta,L)\neq\lim_{\beta\searrow\beta_c}\frac{\partial^2}{\partial\beta^2}\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}}\frac{1}{L^d}\log\mathcal{P}(\beta,L).$$

Though the physical interpretation might not be straightforward, this is a phenomenon caused by the interaction. In fact if $U=0$, $\beta\mapsto\lim_{L\to\infty,L\in\mathbb{N}}\frac{1}{L^d}\log\mathcal{P}(\beta,L)$ is real analytic in $\mathbb{R}_{>0}$. More generally we can deduce a jump discontinuity of

$$\frac{\partial^2}{\partial\beta^2}\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}}\frac{1}{L^d}\log\left(\sum_{n=-bL^d}^{bL^d}e^{it\frac{n}{2}}P_L\left(\frac{n}{2}\right)\right)$$

with β for any $t\in\mathbb{R}$ close to 2π from our previous results.

In [1], [9] the Gärtner-Ellis theorem on large deviation principle was applied to study the rate functions of work distribution functions. So we should report what we can obtain by directly applying the Gärtner-Ellis theorem to our model under the weak coupling condition (1.13). Let $\mathcal{B}(\mathbb{R})$ denote the Borel algebra of $\mathbb{R}$. For $L\in\mathbb{N}$ we define a function $\mu_L:\mathcal{B}(\mathbb{R})\to\mathbb{R}$ by

$$\mu_L(B):=\sum_{n=-bL^d}^{bL^d}1_{\frac{n}{2bL^d}\in B}P_L\left(\frac{n}{2}\right).$$

We see that μ_L is a probability measure on $\mathbb{R}$. Moreover by (1.18) for any $t\in\mathbb{R}$

$$\int_{\mathbb{R}}e^{bL^dtx}d\mu_L(x)=\sum_{n=-bL^d}^{bL^d}e^{t\frac{n}{2}}P_L\left(\frac{n}{2}\right)=\sum_{n=-bL^d}^{bL^d}\frac{\mathrm{Tr}_n\,e^{-\beta\mathsf{H}+t\mathsf{S}_z}}{\mathrm{Tr}\,e^{-\beta\mathsf{H}}}=\frac{\mathrm{Tr}\,e^{-\beta\mathsf{H}+t\mathsf{S}_z}}{\mathrm{Tr}\,e^{-\beta\mathsf{H}}}.$$

One can follow the early derivation of the free energy density of the BCS model [2, Chapter 3] to derive that

$$\begin{aligned}(1.19)\quad &\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}}\frac{1}{L^d}\log\mathrm{Tr}\,e^{-\beta\mathsf{H}+t\mathsf{S}_z}\\ &=D_d\int_{\Gamma_\infty^*}d\mathbf{k}\left(\mathrm{Tr}\log\left(\cosh\left(\frac{t}{2}\right)+\cosh(\beta E(\mathbf{k}))\right)+\mathrm{Tr}\log(2e^{-\beta E(\mathbf{k})})\right).\end{aligned}$$

We should remark that since we assume (1.13), the corresponding gap equation

(1.20)

$$-\frac{2}{|U|}+D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{\sinh(\beta\sqrt{E(\mathbf{k})^2+\Delta^2})}{(\cosh(\frac{t}{2})+\cosh(\beta\sqrt{E(\mathbf{k})^2+\Delta^2}))\sqrt{E(\mathbf{k})^2+\Delta^2}}\right)=0$$

does not have a positive solution. Indeed

$$\begin{aligned}(\text{the R.H.S of (1.20)})&\le-\frac{2}{|U|}+D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{\sqrt{E(\mathbf{k})^2+\Delta^2}}\right)\\ &\le-\frac{2}{|U|}+\frac{b}{e_{min}}<0\end{aligned}$$

for any $\Delta \in \mathbb{R}_{\ge 0}$. This is why the free energy density (1.19) is the same as that of the non-interacting model. Therefore

(1.21)
$$\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}} \frac{1}{bL^d} \log\left(\int_{\mathbb{R}} e^{bL^d tx} d\mu_L(x)\right) = \frac{D_d}{b}\int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\log\left(\frac{\cosh(\frac{t}{2}) + \cosh(\beta E(\mathbf{k}))}{1+\cosh(\beta E(\mathbf{k}))}\right),$$

which is real analytic with t in $\mathbb{R}$. Let us define the function $\Lambda_\beta : \mathbb{R} \to \mathbb{R}$ by the right-hand side of (1.21). It follows from the Gärtner-Ellis theorem (see, e.g., [4]) that for any $u,\, v \in [-\frac{1}{2}, \frac{1}{2}]$ with $u < v$

$$(1.22)\qquad \begin{aligned}\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}} \frac{1}{bL^d} \log\left(\sum_{n=-bL^d}^{bL^d} 1_{\frac{n}{2bL^d}\in[u,v]} P_L\left(\frac{n}{2}\right)\right) &= \lim_{\substack{L\to\infty\\ L\in\mathbb{N}}} \frac{1}{bL^d}\log \mu_L([u,v]) \\ &= -\min_{x\in[u,v]} r(x,\beta),\end{aligned}$$

where the function $r : \mathbb{R}\times\mathbb{R}_{>0} \to \mathbb{R}\cup\{+\infty\}$ is the Legendre transform of Λ_β, i.e.

$$r(x,\beta) := \sup_{t\in\mathbb{R}}(xt - \Lambda_\beta(t)).$$

In fact we can characterize the function $r(\cdot)$ as follows. For any $\beta \in \mathbb{R}_{>0}$

$$\begin{aligned}
&r(x,\beta) = r(-x,\beta),\ \forall x\in\mathbb{R},\\
&r(x,\beta) = +\infty,\ \forall x \in \left(\frac{1}{2},\infty\right),\\
&r\left(\frac{1}{2},\beta\right) = \frac{D_d}{b}\int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\log(2(1+\cosh(\beta E(\mathbf{k})))),\ r(0,\beta) = 0,\\
&\frac{\partial^2 r}{\partial x^2}(x,\beta) > 0,\ \forall x\in\left(-\frac{1}{2},\frac{1}{2}\right),\\
&\frac{\partial r}{\partial x}(x,\beta) < 0,\ \forall x\in\left(-\frac{1}{2},0\right),\ \frac{\partial r}{\partial x}(0,\beta) = 0,\ \frac{\partial r}{\partial x}(x,\beta) > 0,\ \forall x \in \left(0,\frac{1}{2}\right).
\end{aligned}$$

Moreover, $(x,\beta) \mapsto r(x,\beta)$ is real analytic in $(-\frac{1}{2},\frac{1}{2})\times\mathbb{R}_{>0}$, which means that the rate function $r(\cdot,\cdot)$ does not exhibit any singular behavior with the temperature. Despite that DQPTs are triggered by the weak BCS interaction, the interaction plays no role in the rate function. Thus the simple application of the Gärtner-Ellis theorem is unlikely to provide an interpretation of DQPT in terms of the work distribution function.

2 Convexity of the phase boundary

In this section we prove Proposition 1.6. Let us begin by transforming $\frac{d^2\tau}{d\beta^2}(\beta)$ into a form without derivatives of $\tau(\cdot)$. Take any $E \in \mathcal{E}(e_{min}, e_{max})$. Define the function $F : \mathbb{R}_{>0}\times(-1,0) \to \mathbb{R}$ by

$$(2.1)\qquad F(x,y) := D_d\int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{\sinh(xE(\mathbf{k}))}{(y+\cosh(xE(\mathbf{k})))E(\mathbf{k})}\right).$$

Our proof is based on the following equality.

Lemma 2.1. *Let* $U \in [-\frac{2e_{min}}{b}, 0)$.

$$
\begin{aligned}
\frac{d^2\tau}{d\beta^2}(\beta) = &-\frac{2y(\beta)}{(1-y(\beta)^2)^{\frac{3}{2}}}\left(\frac{F_x(\beta, y(\beta))}{F_y(\beta, y(\beta))}\right)^2 \\
&+\frac{2}{(1-y(\beta)^2)^{\frac{1}{2}}F_y(\beta, y(\beta))^3} \\
&\cdot\big(F_{xx}(\beta, y(\beta))F_y(\beta, y(\beta))^2 - 2F_x(\beta, y(\beta))F_y(\beta, y(\beta))F_{xy}(\beta, y(\beta)) \\
&\quad + F_{yy}(\beta, y(\beta))F_x(\beta, y(\beta))^2\big)
\end{aligned}
\tag{2.2}
$$

for any $\beta \in (0, \beta_c)$*, where* $y(\beta) := \cos(\frac{\tau(\beta)}{2})$*,* $F_x(x, y) := \frac{\partial F}{\partial x}(x, y)$ *and other partial derivatives of* F *are abbreviated similarly.*

Proof. We can derive from the equality $-\frac{2}{|U|} + F(\beta, y(\beta)) = 0$ that

$$
\frac{dy}{d\beta}(\beta) = -\frac{F_x(\beta, y(\beta))}{F_y(\beta, y(\beta))}. \tag{2.3}
$$

Because $y \mapsto F(x, y) : (-1, 0) \to \mathbb{R}$ is monotonic, $F_y(\beta, y(\beta)) \neq 0$ for any $\beta \in (0, \beta_c)$. By substituting (2.3)

$$
\frac{d\tau}{d\beta}(\beta) = -\frac{2\frac{dy}{d\beta}(\beta)}{(1-y(\beta)^2)^{\frac{1}{2}}} = \frac{2}{(1-y(\beta)^2)^{\frac{1}{2}}}\cdot\frac{F_x(\beta, y(\beta))}{F_y(\beta, y(\beta))}.
$$

By differentiating both sides with β and substituting (2.3) again we can obtain the claimed equality. ☐

In the rest of this paper we often let $y(\beta)$ denote $\cos(\frac{\tau(\beta)}{2})$ without any remark. The next lemma means that for any e_{min}, e_{max} satisfying $0 < e_{min} \le e_{max}$, $\beta \in (0, \beta_c)$ sufficiently close to β_c $\frac{d^2\tau}{d\beta^2}(\beta) > 0$.

Lemma 2.2. *There exists* $M(e_{min}, e_{max}) \in \mathbb{R}_{>0}$ *depending only on* e_{min}*,* e_{max} *such that for any* $U \in [-\frac{e_{min}}{\sinh(2)b}, 0)$*,* $E \in \mathcal{E}(e_{min}, e_{max})$*,* $\beta \in (0, \beta_c)$ *satisfying* $\beta \ge M(e_{min}, e_{max})\sqrt{1 + y(\beta)}$

$$
\frac{d^2\tau}{d\beta^2}(\beta) \ge \frac{\beta^2}{4(1+y(\beta))^{\frac{3}{2}}}\left(\frac{e_{max}e_{min}}{\sinh(2e_{max}/e_{min})}\right)^2.
$$

Since $\lim_{\beta \nearrow \beta_c} y(\beta) = -1$ by Lemma 1.2, we can deduce the following statement from the above lemma.

Corollary 2.3. *For any* $U \in [-\frac{e_{min}}{\sinh(2)b}, 0)$*,* $E \in \mathcal{E}(e_{min}, e_{max})$

$$
\lim_{\beta \nearrow \beta_c} \frac{d^2\tau}{d\beta^2}(\beta) = +\infty.
$$

From time to time we will need explicit forms of the partial derivatives of F. Let us list them here.

$$
F_x(x, y) = D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1 + y\cosh(xE(\mathbf{k}))}{(y + \cosh(xE(\mathbf{k})))^2}\right), \tag{2.4}
$$

(2.5) $$F_y(x,y) = -D_d \int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{\sinh(xE(\mathbf{k}))}{(y+\cosh(xE(\mathbf{k})))^2 E(\mathbf{k})}\right),$$

(2.6) $$F_{xx}(x,y) = D_d \int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{E(\mathbf{k})\sinh(xE(\mathbf{k}))(y^2 - y\cosh(xE(\mathbf{k})) - 2)}{(y+\cosh(xE(\mathbf{k})))^3}\right),$$

(2.7) $$F_{xy}(x,y) = D_d \int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{\cosh^2(xE(\mathbf{k})) - y\cosh(xE(\mathbf{k})) - 2}{(y+\cosh(xE(\mathbf{k})))^3}\right),$$

(2.8) $$F_{yy}(x,y) = 2D_d \int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{\sinh(xE(\mathbf{k}))}{(y+\cosh(xE(\mathbf{k})))^3 E(\mathbf{k})}\right).$$

We will use the following properties in the proof of Lemma 2.2. In fact these were derived in the proof of [13, Proposition 2.8]. We show them again for readers' convenience.

Lemma 2.4. *Let $U \in [-\frac{e_{min}}{\sinh(2)b}, 0)$. Then the following inequalities hold.*

$$\begin{aligned}
&\beta_c \le \frac{2}{e_{min}}.\\
&y(\beta)+1 \le \frac{b\sinh(2)|U|}{2e_{min}},\ \forall\beta\in(0,\beta_c).\\
&-y(\beta) \ge \frac{1}{2},\ \forall\beta\in(0,\beta_c).
\end{aligned}$$

Proof. By Lemma 1.1

$$\begin{aligned}
\beta_c &\le \frac{2}{e_{min}}\tanh^{-1}\left(\frac{b|U|}{2e_{min}}\right) \le \frac{2}{e_{min}}\tanh^{-1}\left(\frac{1}{2\sinh(2)}\right) \le \frac{2}{e_{min}}\tanh^{-1}(\tanh(1))\\
&= \frac{2}{e_{min}}.
\end{aligned}$$

It follows from the above inequality, the equality $-\frac{2}{|U|} + F(\beta, y(\beta)) = 0$ and the property (1.17) that

$$\frac{2}{|U|} \le \frac{b\sinh(\beta e_{min})}{(y(\beta)+\cosh(\beta e_{min}))e_{min}} \le \frac{b\sinh(2)}{(y(\beta)+\cosh(\beta e_{min}))e_{min}},$$

or by the assumption

$$y(\beta)+1 \le y(\beta)+\cosh(\beta e_{min}) \le \frac{b\sinh(2)|U|}{2e_{min}} \le \frac{1}{2}.$$

This implies the second and the third inequality. □

Proof of Lemma 2.2. Let us establish necessary inequalities by assuming that $\beta \ge M\sqrt{1+y(\beta)}$ with $M \in \mathbb{R}_{>0}$. We will tune M afterwards. It follows that

(2.9) $$-y(\beta) \ge 1 - \frac{\beta^2}{M^2}.$$

By (2.4) and (2.9)

$$-F_x(\beta, y(\beta))$$

$$
\begin{aligned}
&\geq D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{(1-\beta^2/M^2)\cosh(\beta E(\mathbf{k}))-1}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right)\\
&\geq \left(\frac{\beta^2}{2}e_{min}^2 - \frac{\beta^2}{M^2}\cosh(\beta e_{max})\right) D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right)\\
&\geq \beta^2 \left(\frac{1}{2}e_{min}^2 - \frac{1}{M^2}\cosh(\beta_c e_{max})\right) D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right).
\end{aligned}
$$

By (2.5)

$$
0 < -F_y(\beta, y(\beta)) \leq \frac{\sinh(\beta e_{max})}{e_{max}} D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right).
$$

Thus by assuming that

$$
\frac{1}{2}e_{min}^2 - \frac{1}{M^2}\cosh(\beta_c e_{max}) > 0 \tag{2.10}
$$

$$
\begin{aligned}
\left(\frac{F_x(\beta, y(\beta))}{F_y(\beta, y(\beta))}\right)^2 &\geq \beta^2 \left(\frac{\beta e_{max}}{\sinh(\beta e_{max})}\left(\frac{1}{2}e_{min}^2 - \frac{1}{M^2}\cosh(\beta_c e_{max})\right)\right)^2\\
&\geq \beta^2 \left(\frac{\beta_c e_{max}}{\sinh(\beta_c e_{max})}\left(\frac{1}{2}e_{min}^2 - \frac{1}{M^2}\cosh(\beta_c e_{max})\right)\right)^2.
\end{aligned} \tag{2.11}
$$

To bound $|F_{xx}(\beta, y(\beta))|$, observe that since $y(\beta) \in (-1, 0)$,

$$
\begin{aligned}
|y(\beta)^2 - y(\beta)\cosh(\beta\alpha) - 2| &= |(y(\beta)-2)(y(\beta)+1) + y(\beta)(1-\cosh(\beta\alpha))|\\
&\leq 3(y(\beta)+1) + \cosh(\beta\alpha) - 1 \leq 3(y(\beta)+\cosh(\beta\alpha))
\end{aligned}
$$

for any $\alpha \in \mathbb{R}$. Therefore

$$
|F_{xx}(\beta, y(\beta))| \leq 3D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{E(\mathbf{k})\sinh(\beta E(\mathbf{k}))}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right) \leq 3e_{max}^2 |F_y(\beta, y(\beta))|,
$$

or

$$
\left|\frac{F_{xx}(\beta, y(\beta))}{F_y(\beta, y(\beta))}\right| \leq 3e_{max}^2. \tag{2.12}
$$

Moreover, since

$$
\begin{aligned}
|1 + y(\beta)\cosh(\beta\alpha)| &= |1 + y(\beta) + y(\beta)(\cosh(\beta\alpha)-1)| \leq 1 + y(\beta) + \cosh(\beta\alpha) - 1\\
&= y(\beta) + \cosh(\beta\alpha)
\end{aligned} \tag{2.13}
$$

for any $\alpha \in \mathbb{R}$,

$$
|F_x(\beta, y(\beta))| \leq (y(\beta) + \cosh(\beta e_{max})) D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right). \tag{2.14}
$$

Also,

$$
|F_y(\beta, y(\beta))| \geq \beta D_d \int_{\Gamma^*_\infty} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{(y(\beta)+\cosh(\beta E(\mathbf{k})))^2}\right). \tag{2.15}
$$

To bound $|F_{xy}(\beta, y(\beta))|$, we remark that for any $\alpha \in \mathbb{R}$

$$
\begin{aligned}
&|\cosh^2(\beta\alpha) - y(\beta)\cosh(\beta\alpha) - 2| \\
&= |(\cosh(\beta\alpha) - 1)^2 + 2(\cosh(\beta\alpha) - 1) - 1 - y(\beta)\cosh(\beta\alpha)| \\
&\leq |(\cosh(\beta\alpha) - 1)^2 + 2(\cosh(\beta\alpha) - 1)| + y(\beta) + \cosh(\beta\alpha) \\
&\leq (\cosh(\beta\alpha) + y(\beta))(\cosh(\beta\alpha) + 2).
\end{aligned}
$$

In the 1st inequality we used (2.13). Thus

$$
|F_{xy}(\beta, y(\beta))| \leq (\cosh(\beta_c e_{max}) + 2) D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{(y(\beta) + \cosh(\beta E(\mathbf{k})))^2}\right). \tag{2.16}
$$

By combining (2.14), (2.15), (2.16) with (2.9)

$$
\begin{aligned}
\left|\frac{F_x(\beta, y(\beta))F_{xy}(\beta, y(\beta))}{F_y(\beta, y(\beta))^2}\right| &\leq \beta^{-2}(y(\beta) + \cosh(\beta e_{max}))(\cosh(\beta_c e_{max}) + 2) \\
&\leq \beta^{-2}\left(\frac{\beta^2}{M^2} + \cosh(\beta e_{max}) - 1\right)(\cosh(\beta_c e_{max}) + 2) \\
&\leq \left(\frac{1}{M^2} + \frac{\cosh(\beta_c e_{max}) - 1}{\beta_c^2}\right)(\cosh(\beta_c e_{max}) + 2).
\end{aligned} \tag{2.17}
$$

One can deduce that

$$
|F_{yy}(\beta, y(\beta))| \leq \frac{2}{y(\beta) + \cosh(\beta e_{min})}|F_y(\beta, y(\beta))|. \tag{2.18}
$$

It follows from (2.14), (2.15), (2.18) and (2.9) that

$$
\begin{aligned}
\left|\frac{F_{yy}(\beta, y(\beta))F_x(\beta, y(\beta))^2}{F_y(\beta, y(\beta))^3}\right| &\leq \frac{2}{y(\beta) + \cosh(\beta e_{min})}\left(\frac{F_x(\beta, y(\beta))}{F_y(\beta, y(\beta))}\right)^2 \\
&\leq \frac{2(y(\beta) + \cosh(\beta e_{max}))^2}{\beta^2(y(\beta) + \cosh(\beta e_{min}))} \leq \frac{2(\frac{\beta^2}{M^2} + \cosh(\beta e_{max}) - 1)^2}{\beta^2(\cosh(\beta e_{min}) - 1)} \\
&\leq \frac{4}{e_{min}^2}\left(\frac{1}{M^2} + \frac{\cosh(\beta_c e_{max}) - 1}{\beta_c^2}\right)^2.
\end{aligned} \tag{2.19}
$$

By substituting (2.11), (2.12), (2.17), (2.19) into the right-hand side of (2.2) we have that

$$
\begin{aligned}
&(1 + y(\beta))^{\frac{3}{2}}\frac{d^2\tau}{d\beta^2}(\beta) \\
&\geq -\frac{2y(\beta)}{(1 - y(\beta))^{\frac{3}{2}}}\beta^2\left(\frac{\beta_c e_{max}}{\sinh(\beta_c e_{max})}\left(\frac{e_{min}^2}{2} - \frac{1}{M^2}\cosh(\beta_c e_{max})\right)\right)^2 \\
&\quad - \frac{2\beta^2}{\sqrt{1 - y(\beta)}M^2}\left(3e_{max}^2 + 2\left(\frac{1}{M^2} + \frac{\cosh(\beta_c e_{max}) - 1}{\beta_c^2}\right)(\cosh(\beta_c e_{max}) + 2)\right. \\
&\qquad\qquad \left. + \frac{4}{e_{min}^2}\left(\frac{1}{M^2} + \frac{\cosh(\beta_c e_{max}) - 1}{\beta_c^2}\right)^2\right).
\end{aligned}
$$

Here we also used that

$$\frac{2(1+y(\beta))}{\sqrt{1-y(\beta)}} \le \frac{2\beta^2}{\sqrt{1-y(\beta)}M^2}.$$

Then by assuming

$$\frac{e_{min}^2}{2} - \frac{1}{M^2}\cosh\left(\frac{2e_{max}}{e_{min}}\right) > 0 \tag{2.20}$$

and substituting the inequalities claimed in Lemma 2.4

(2.21)

$$\begin{aligned}&(1+y(\beta))^{\frac{3}{2}}\frac{d^2\tau}{d\beta^2}(\beta)\\ &\ge \frac{\beta^2}{2\sqrt{2}}\left(\frac{2e_{max}}{e_{min}\sinh(2e_{max}/e_{min})}\left(\frac{e_{min}^2}{2} - \frac{1}{M^2}\cosh\left(\frac{2e_{max}}{e_{min}}\right)\right)\right)^2\\ &\quad - \frac{2\beta^2}{M^2}\left(3e_{max}^2 + 2\left(\frac{1}{M^2} + \frac{e_{min}^2}{4}\left(\cosh\left(\frac{2e_{max}}{e_{min}}\right) - 1\right)\right)\left(\cosh\left(\frac{2e_{max}}{e_{min}}\right) + 2\right)\right.\\ &\qquad\qquad \left. + \frac{4}{e_{min}^2}\left(\frac{1}{M^2} + \frac{e_{min}^2}{4}\left(\cosh\left(\frac{2e_{max}}{e_{min}}\right) - 1\right)\right)^2\right).\end{aligned}$$

Note that (2.20) holds for sufficiently large M and implies (2.10). Moreover, $\frac{1}{\beta^2}$(R.H.S of (2.21)) is independent of β and

$$\lim_{M\to\infty}\frac{1}{\beta^2}(\text{R.H.S of (2.21)}) = \frac{1}{2\sqrt{2}}\left(\frac{e_{max}e_{min}}{\sinh(2e_{max}/e_{min})}\right)^2.$$

Thus we can choose $M(e_{min}, e_{max}) \in \mathbb{R}_{>0}$ depending only on e_{min}, e_{max} so that the claim of the lemma holds. ☐

The inequality $\beta \ge M(e_{min}, e_{max})\sqrt{1+y(\beta)}$ does not hold for small β.

Lemma 2.5. *For any $E \in \mathcal{E}(e_{min}, e_{max})$, $U \in (-\frac{2e_{min}}{b}, 0)$*

$$\lim_{\beta\searrow 0}\frac{\beta}{\sqrt{1+y(\beta)}} = 0.$$

Proof. By (1.17)

$$\frac{\beta^2}{y(\beta)+\cosh(\beta e_{max})} \le \beta D_d\int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{\sinh(\beta E(\mathbf{k}))}{(y(\beta)+\cosh(\beta E(\mathbf{k})))E(\mathbf{k})}\right) = \frac{2\beta}{|U|}.$$

Thus

$$\lim_{\beta\searrow 0}\frac{\beta^2}{y(\beta)+\cosh(\beta e_{max})} = 0,$$

which implies the claim. ☐

Remark 2.6. In the proof of [13, Lemma 2.2] we proved more precisely that

$$\lim_{\beta\searrow 0}\frac{y(\beta)+1}{\beta}=\frac{b|U|}{2}$$

by a longer argument.

Therefore Lemma 2.2 does not prove the positivity of $\frac{d^2\tau}{d\beta^2}(\beta)$ for small β. We must prove the positivity in case that $\beta < M(e_{min}, e_{max})\sqrt{1+y(\beta)}$. In the rest of this section we achieve this as follows. We show by scaling that the right-hand side of (2.2) is close to a function independent of $y(\beta)$, which proves to be positive if $\frac{e_{min}}{e_{max}} > \sqrt{9-4\sqrt{5}}$.

Let us construct the proof step by step. For $x \in \mathbb{R}_{>0}$, $y \in (-1, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$ we set

$$\begin{aligned}(2.22)\quad W_E(x,y) := &\frac{2}{(1-y)^{\frac{3}{2}}\big((y+1)^{\frac{3}{2}}F_y(\sqrt{y+1}x,y)/x\big)^3}\Bigg(\\
&-y\big((y+1)F_x(\sqrt{y+1}x,y)\big)^2\frac{(y+1)^{\frac{3}{2}}}{x}F_y(\sqrt{y+1}x,y)\\
&+(1-y)\Bigg(2\left(\frac{x(y+1)^{\frac{3}{2}}}{2}F_{xx}(\sqrt{y+1}x,y)\right)\left(\frac{(y+1)^{\frac{3}{2}}}{x}F_y(\sqrt{y+1}x,y)\right)^2\\
&\quad-2\big((y+1)F_x(\sqrt{y+1}x,y)\big)\left(\frac{(y+1)^{\frac{3}{2}}}{x}F_y(\sqrt{y+1}x,y)\right)\\
&\quad\cdot\big((y+1)^2F_{xy}(\sqrt{y+1}x,y)\big)\\
&\quad+\left(\frac{(y+1)^{\frac{5}{2}}}{x}F_{yy}(\sqrt{y+1}x,y)\right)\big((y+1)F_x(\sqrt{y+1}x,y)\big)^2\Bigg)\Bigg).\end{aligned}$$

We can see from (2.2) that

$$(2.23)\qquad \frac{\beta^2}{\sqrt{1+y(\beta)}}\frac{d^2\tau}{d\beta^2}(\beta)=W_E\left(\frac{\beta}{\sqrt{1+y(\beta)}},y(\beta)\right),\ \forall\beta\in(0,\beta_c).$$

Since $\lim_{x\searrow 0}F_y(\sqrt{y+1}x,y)/x$ converges to a non-zero value and $\lim_{x\searrow 0}F_{yy}(\sqrt{y+1}x,y)/x$ converges in particular, $\lim_{x\searrow 0}W_E(x,y)$ converges for any $y\in(-1,0)$. Thus in the following we consider $W_E(\cdot,\cdot)$ as a continuous function on $\mathbb{R}_{\ge 0}\times(-1,0)$. For $y\in(-1,0)$ close to -1 $W_E(x,y)$ can be approximated by $\tilde{W}_E(x)$ defined by

(2.24)

$$\begin{aligned}\tilde{W}_E(x) :=&\frac{D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{1+\frac{x^2}{2}E(\mathbf{k})^2}\right)}{\sqrt{2}\left(D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^2}\right)\right)^3}\Bigg(\\
&4\left(D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^2}\right)\right)^2\\
&+D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{1+\frac{x^2}{2}E(\mathbf{k})^2}\right)D_d\int_{\Gamma_\infty^*}d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^2}\right)\end{aligned}$$

$$- 4D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{1}{1+\frac{x^2}{2}E(\mathbf{k})^2}\right) D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^3}\right)\Bigg).$$

We can consider $\tilde{W}_E(\cdot)$ as a continuous function on $\mathbb{R}_{\geq 0}$.

Lemma 2.7. *For any $r \in \mathbb{R}_{>0}$*

$$\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} |W_E(x,y) - \tilde{W}_E(x)| = 0.$$

Proof. For $E \in \mathcal{E}(e_{min}, e_{max})$ we define the functions $\tilde{F}^{(x)}$, $\tilde{F}^{(y)}$, $\tilde{F}^{(xx)}$, $\tilde{F}^{(xy)}$, $\tilde{F}^{(yy)}(\in C(\mathbb{R}_{\geq 0}))$ by

$$\begin{aligned}
\tilde{F}^{(x)}(x) &:= D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{1-\frac{x^2}{2}E(\mathbf{k})^2}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^2}\right), \\
\tilde{F}^{(y)}(x) &:= -D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^2}\right), \\
\tilde{F}^{(xx)}(x) &:= D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{\frac{x^2}{2}E(\mathbf{k})^2(-3+\frac{x^2}{2}E(\mathbf{k})^2)}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^3}\right), \\
\tilde{F}^{(xy)}(x) &:= D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{\frac{3}{2}x^2E(\mathbf{k})^2-1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^3}\right), \\
\tilde{F}^{(yy)}(x) &:= D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr}\left(\frac{2}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^3}\right).
\end{aligned}$$

By using (1.10), (1.11) we can prove that for any $r \in \mathbb{R}_{>0}$

$$\begin{aligned}
&\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} |(y+1)F_x(\sqrt{y+1}x, y) - \tilde{F}^{(x)}(x)| = 0, \\
&\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} \left|\frac{(y+1)^{\frac{3}{2}}}{x}F_y(\sqrt{y+1}x, y) - \tilde{F}^{(y)}(x)\right| = 0, \\
&\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} \left|\frac{x(y+1)^{\frac{3}{2}}}{2}F_{xx}(\sqrt{y+1}x, y) - \tilde{F}^{(xx)}(x)\right| = 0, \\
&\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} |(y+1)^2F_{xy}(\sqrt{y+1}x, y) - \tilde{F}^{(xy)}(x)| = 0, \\
&\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} \left|\frac{(y+1)^{\frac{5}{2}}}{x}F_{yy}(\sqrt{y+1}x, y) - \tilde{F}^{(yy)}(x)\right| = 0.
\end{aligned}$$

Since

$$|\tilde{F}^{(y)}(x)| \geq \frac{b}{(1+\frac{x^2}{2}e_{max}^2)^2}$$

for any $x \in \mathbb{R}_{\geq 0}$ and $E \in \mathcal{E}(e_{min}, e_{max})$, we can justify that for any $r \in \mathbb{R}_{>0}$

$$\lim_{y \searrow -1} \sup_{\substack{x\in[0,r] \\ E\in\mathcal{E}(e_{min},e_{max})}} |W_E(x,y) - \hat{W}_E(x)| = 0,$$

where

(2.25)

$$\hat{W}_E(x) := \frac{1}{\sqrt{2}(\tilde{F}^{(y)}(x))^3}\Big((\tilde{F}^{(x)}(x))^2\tilde{F}^{(y)}(x) + 2\left(2\tilde{F}^{(xx)}(x)(\tilde{F}^{(y)}(x))^2 - 2\tilde{F}^{(x)}(x)\tilde{F}^{(y)}(x)\tilde{F}^{(xy)}(x) + \tilde{F}^{(yy)}(x)(\tilde{F}^{(x)}(x))^2\right)\Big).$$

By setting

$$\tilde{F}_n := D_d\int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(\frac{1}{(1+\frac{x^2}{2}E(\mathbf{k})^2)^n}\right)\ (n\in\mathbb{N})$$

we have that

$$\tilde{F}^{(x)}(x) = 2\tilde{F}_2 - \tilde{F}_1,\ \tilde{F}^{(y)}(x) = -\tilde{F}_2,\ \tilde{F}^{(xx)}(x) = \tilde{F}_1 - 5\tilde{F}_2 + 4\tilde{F}_3,$$
$$\tilde{F}^{(xy)}(x) = 3\tilde{F}_2 - 4\tilde{F}_3,\ \tilde{F}^{(yy)}(x) = 2\tilde{F}_3.$$

By substituting these into the right-hand side of (2.25) we can derive that $\hat{W}_E(x) = \tilde{W}_E(x)$ for $x\in\mathbb{R}_{\geq 0}$, which completes the proof. □

Based on (2.23) and Lemma 2.7, we can partially achieve the goal.

Lemma 2.8. *Let $M(e_{min},e_{max})$ be the (e_{min},e_{max})-dependent constant introduced in Lemma 2.2. Assume that*

$$\inf_{\substack{x\in[0,M(e_{min},e_{max})]\\ E\in\mathcal{E}(e_{min},e_{max})}} \tilde{W}_E(x) > 0. \tag{2.26}$$

Then there exists $U_0\in(0,\frac{e_{min}}{\sinh(2)b}]$ such that for any $U\in[-U_0,0)$, $E\in\mathcal{E}(e_{min},e_{max})$, $\beta\in(0,\beta_c)$ satisfying $\beta\leq M(e_{min},e_{max})\sqrt{1+y(\beta)}$

$$\frac{d^2\tau}{d\beta^2}(\beta) \geq \frac{\sqrt{1+y(\beta)}}{2\beta^2}\tilde{W}_E\left(\frac{\beta}{\sqrt{1+y(\beta)}}\right).$$

Proof. By Lemma 2.7 and the assumption there exists $y_0\in(-1,0)$ such that for any $x\in[0,M(e_{min},e_{max})]$, $y\in(-1,y_0]$, $E\in\mathcal{E}(e_{min},e_{max})$

$$W_E(x,y) \geq \frac{1}{2}\tilde{W}_E(x). \tag{2.27}$$

By the 2nd inequality of Lemma 2.4 there exists $U_0\in(0,\frac{e_{min}}{\sinh(2)b}]$ such that for any $U\in[-U_0,0)$, $E\in\mathcal{E}(e_{min},e_{max})$, $\beta\in(0,\beta_c)$ $y(\beta)\in(-1,y_0]$. Combination of this property with (2.23), (2.27) ensures the claim. □

It remains to prove (2.26). Observe that for $E\in\mathcal{E}(e_{min},e_{max})$, $n\in\mathbb{N}$

$$D_d\int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}\left(1+\frac{x^2}{2}E(\mathbf{k})^2\right)^{-n} = (2\pi)^{-d}\int_{[0,2\pi]^d} d\hat{\mathbf{k}}\,\mathrm{Tr}\left(1+\frac{x^2}{2}E\left(\sum_{j=1}^d \hat{k}_j\hat{\mathbf{v}}_j\right)^2\right)^{-n}$$

$$= \lim_{N\to\infty} N^{-d} \prod_{j=1}^{d} \left(\sum_{n_j=0}^{N-1} \right) \mathrm{Tr} \left(1 + \frac{x^2}{2} E \left(\frac{2\pi}{N} \sum_{j=1}^{d} n_j \hat{\mathbf{v}}_j \right)^2 \right)^{-n} .$$

Moreover for any $N \in \mathbb{N}$ there exist $M \in \mathbb{N}$, $(s_j)_{j=1}^M \in \mathbb{R}_{>0}^M$ satisfying $\sum_{j=1}^M s_j = 1$, $(e_j)_{j=1}^M \in \mathbb{R}_{>0}^M$ satisfying $e_{min} \le e_1 < \cdots < e_M \le e_{max}$ such that

$$N^{-d} \prod_{j=1}^{d} \left(\sum_{n_j=0}^{N-1} \right) \mathrm{Tr} \left(1 + \frac{x^2}{2} E \left(\frac{2\pi}{N} \sum_{j=1}^{d} n_j \hat{\mathbf{v}}_j \right)^2 \right)^{-n} = b \sum_{j=1}^{M} s_j \left(1 + \frac{x^2}{2} e_j^2 \right)^{-n} .$$

For conciseness let us set

$$X := \frac{x^2}{2},$$
$$\mathbb{S}(M) := \left\{ (s_j)_{j=1}^M \in \mathbb{R}_{>0}^M \;\middle|\; \sum_{j=1}^{M} s_j = 1 \right\},$$
$$\mathbb{A}(M) := \{ (A_j)_{j=1}^M \in \mathbb{R}_{>0}^M \mid e_{min}^2 \le A_1 < \cdots < A_M \le e_{max}^2 \}$$

for $M \in \mathbb{N}$ and

$$C_n := \sum_{j=1}^{M} s_j (1 + X A_j)^{-n}$$

for $n \in \mathbb{N}$, $(s_j)_{j=1}^M \in \mathbb{S}(M)$, $(A_j)_{j=1}^M \in \mathbb{A}(M)$. We do not indicate the dependency of C_n on X, M, $(s_j)_{j=1}^M$, $(A_j)_{j=1}^M$ for simplicity. By the definition (2.24)

$$\tilde{W}_E(x) \ge \inf_{M\in\mathbb{N}} \inf_{(s_j)_{j=1}^M \in \mathbb{S}(M)} \inf_{(A_j)_{j=1}^M \in \mathbb{A}(M)} \inf_{X \in \mathbb{R}_{\ge 0}} \frac{C_1}{\sqrt{2} C_2^3} (4C_2^2 + C_1 C_2 - 4 C_1 C_3) \tag{2.28}$$

for any $x \in \mathbb{R}_{\ge 0}$, $E \in \mathcal{E}(e_{min}, e_{max})$. Thus it suffices to prove that the right-hand side of (2.28) is positive. In fact we can prove the following.

Lemma 2.9. *Assume that* $\frac{e_{min}}{e_{max}} \ge \sqrt{9 - 4\sqrt{5}}$. *Then there exists a positive constant* c *independent of any parameter such that*

$$\inf_{M\in\mathbb{N}} \inf_{(s_j)_{j=1}^M \in \mathbb{S}(M)} \inf_{(A_j)_{j=1}^M \in \mathbb{A}(M)} \inf_{X \in \mathbb{R}_{\ge 0}} \frac{C_1}{C_2^3} (4C_2^2 + C_1 C_2 - 4 C_1 C_3)$$
$$\ge c \left(\left(\frac{e_{min}}{e_{max}} \right)^2 - 9 + 4\sqrt{5} \right)^2 .$$

We need to construct tools to prove Lemma 2.9. To shorten subsequent formulas, let us set

$$B_i := \frac{1}{1 + A_i X}, \tag{2.29}$$

$$D_{i,j} := \frac{1}{2} (8 B_i^2 B_j^2 + B_i B_j^2 + B_i^2 B_j - 4 B_i B_j^3 - 4 B_i^3 B_j) \tag{2.30}$$

for A_i, $A_j \in \mathbb{R}_{>0}$ and $X \in \mathbb{R}_{\geq 0}$. The following transformation of $D_{i,j}$ will be useful. For any $\gamma \in \mathbb{R}$

(2.31)
$$D_{i,j} = \frac{1}{2}B_iB_j(2\gamma - (\gamma - B_i) - (\gamma - B_j) - 4(\gamma - B_i)^2 - 4(\gamma - B_j)^2 + 8(\gamma - B_i)(\gamma - B_j)).$$

Lemma 2.10. *For any $M \in \mathbb{N}$, $(s_j)_{j=1}^M \in \mathbb{S}(M)$, $(A_j)_{j=1}^M \in \mathbb{A}(M)$, $X \in \mathbb{R}_{\geq 0}$*

$$4C_2^2 + C_1C_2 - 4C_1C_3 = \langle (s_j)_{j=1}^M, (D_{i,j})_{1\leq i,j\leq M}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M}, \tag{2.32}$$

where $\langle \cdot, \cdot \rangle_{\mathbb{R}^M}$ is the canonical inner product of $\mathbb{R}^M$.

Proof. Observe that

$$\begin{aligned}
&4C_2^2 + C_1C_2 - 4C_1C_3 \\
&= \sum_{i=1}^M \sum_{j=1}^M s_is_j(4B_i^2B_j^2 + B_iB_j^2 - 4B_iB_j^3) \\
&= \sum_{i=1}^M s_i^2B_i^3 + \sum_{i=1}^M \sum_{j=1}^M (1_{i<j} + 1_{i>j})s_is_j(4B_i^2B_j^2 + B_iB_j^2 - 4B_iB_j^3) \\
&= \sum_{i=1}^M s_i^2B_i^3 + \sum_{i=1}^M \sum_{j=1}^M 1_{i<j}s_is_j 2D_{i,j} = \sum_{i=1}^M s_i^2 D_{i,i} + \sum_{i=1}^M \sum_{j=1}^M 1_{i\neq j}s_is_jD_{i,j} \\
&= \langle (s_j)_{j=1}^M, (D_{i,j})_{1\leq i,j\leq M}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M}.
\end{aligned}$$

□

Let us prepare lemmas to find a lower bound on the right-hand side of (2.32). We set for A_1, $A_2 \in \mathbb{R}_{>0}$

$$\alpha(A_1, A_2) := \frac{A_1^{\frac{1}{3}} + A_2^{\frac{1}{3}}}{A_1^{\frac{2}{3}}A_2^{\frac{2}{3}}}. \tag{2.33}$$

We begin with the next lemma from which the critical constant $9-4\sqrt{5}$ originates.

Lemma 2.11. *Assume that $0 < A_1 < A_2$.*

(i) The function $X \mapsto B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}} : \mathbb{R}_{\geq 0} \to \mathbb{R}$ attains its maximum only at $X = \alpha(A_1, A_2)$. Moreover,

$$(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}})|_{X=\alpha(A_1,A_2)} = \frac{1 - (A_1/A_2)^{\frac{1}{3}}}{\sqrt{1 + (A_1/A_2)^{\frac{1}{3}} + (A_1/A_2)^{\frac{2}{3}}}}.$$

(ii) The maximum value $\max_{X\in\mathbb{R}_{\geq 0}}(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}})$ is strictly decreasing with $\frac{A_1}{A_2}$.

(iii) $\max_{X\in\mathbb{R}_{\geq 0}}(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}}) = \frac{1}{2}$ if and only if $\frac{A_1}{A_2} = 9 - 4\sqrt{5}$.

Proof. (i): One can derive that

$$\begin{aligned}
&\frac{d}{dX}(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}}) \\
&= \frac{(A_2^{\frac{1}{3}} - A_1^{\frac{1}{3}})(A_2^{\frac{2}{3}}(1+A_1X) + A_1^{\frac{1}{3}}A_2^{\frac{1}{3}}(1+A_1X)^{\frac{1}{2}}(1+A_2X)^{\frac{1}{2}} + A_1^{\frac{2}{3}}(1+A_2X))}{2(1+A_1X)^{\frac{3}{2}}(1+A_2X)^{\frac{3}{2}}(A_2^{\frac{1}{3}}(1+A_1X)^{\frac{1}{2}} + A_1^{\frac{1}{3}}(1+A_2X)^{\frac{1}{2}})} \\
&\quad \cdot (A_1^{\frac{1}{3}} + A_2^{\frac{1}{3}} - A_1^{\frac{2}{3}}A_2^{\frac{2}{3}}X).
\end{aligned}$$

The claim follows from the above equality. The maximum value can be derived directly.

(ii): One can deduce the claim from (i).

(iii): We can check that

$$\frac{1-(A_1/A_2)^{\frac{1}{3}}}{\sqrt{1+(A_1/A_2)^{\frac{1}{3}}+(A_1/A_2)^{\frac{2}{3}}}} = \frac{1}{2}$$

if and only if $\frac{A_1}{A_2} = 9 - 4\sqrt{5}$. Thus by (i) the claim holds true. $\square$

We need to prove properties of B_i, $D_{i,j}$ more.

Lemma 2.12. *(i) For any $A_1, A_2 \in \mathbb{R}_{>0}$ satisfying $A_1 \le A_2$, $X \in \mathbb{R}_{\ge 0}$*

$$D_{1,1} - D_{1,2} = \frac{1}{2}B_1(B_1 - B_2)(2B_1 + B_2 + 4B_2(B_1 - B_2)).$$

(ii) For any $A_1, A_2 \in \mathbb{R}_{>0}$ satisfying $A_1 \le A_2$, $X \in \mathbb{R}_{\ge 0}$

$$\begin{aligned}
D_{1,1}D_{2,2} - D_{1,2}^2 =& 4B_1^2B_2^2(B_1 - B_2)^2\left(B_1^{\frac{1}{2}} + B_2^{\frac{1}{2}} + \frac{1}{2}\right)\left(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}} + \frac{1}{2}\right) \\
&\cdot \left(\frac{1}{2} - B_1^{\frac{1}{2}} + B_2^{\frac{1}{2}}\right)\left(B_1^{\frac{1}{2}} + B_2^{\frac{1}{2}} - \frac{1}{2}\right).
\end{aligned}$$

(iii) For any $A_1, A_2, A_3, A_4 \in \mathbb{R}_{>0}$ satisfying $A_1 < A_2 \le A_3 \le A_4$, $X \in \mathbb{R}_{>0}$

$$D_{1,1}D_{2,3} - D_{1,2}D_{1,3} \ge \frac{B_2B_3(B_1 - B_2)(B_1 - B_3)}{B_4^2(B_1 - B_4)^2}(D_{1,1}D_{4,4} - D_{1,4}^2).$$

(iv) Assume that $0 < A_1 \le A_2$ and $X \in \mathbb{R}_{\ge 0}$.

$$D_{1,2} \ge D_{2,2} \text{ if and only if } B_1 - B_2 \le \frac{3B_1}{2(2B_1 + 1)}.$$

(v) Assume that $0 < A_1 < A_2$ and $X \in \mathbb{R}_{>0}$.

$$D_{1,2} \le D_{2,2} \text{ if and only if } B_1 - B_2 \ge \frac{3B_1}{2(2B_1 + 1)}.$$

(vi) Let $A_1, A_2, \cdots, A_M \in \mathbb{R}_{>0}$ satisfy $A_1 \le A_2 \le \cdots \le A_M$ and $X \in \mathbb{R}_{\ge 0}$. If $D_{1,M} \ge D_{M,M}$, then $D_{1,m} \ge D_{m,m} \ge D_{M,M}$ for any $m \in \{1, 2, \cdots, M\}$.

(vii) Let $A_1, A_2 \in \mathbb{R}_{>0}$ satisfy $A_1 \le A_2$, $\frac{A_1}{A_2} \ge 9-4\sqrt{5}$ and $X \in \mathbb{R}_{\ge 0}$. If $D_{2,2} \ge D_{1,2}$, there exists $c \in \mathbb{R}_{>0}$ independent of any parameter such that

$$D_{1,1}D_{2,2} - D_{1,2}^2 \ge cB_1^2B_2^2(B_1 - B_2)^2 \left(\frac{A_1}{A_2} - 9 + 4\sqrt{5}\right)^2.$$

Proof. (i), (ii): These can be derived from the definitions. The equality (2.31) with $\gamma = B_1$ helps the derivations.

(iii): Observe that by using (2.31) with $\gamma = B_1$ and the inequalities $B_1 > B_2 \ge B_3 \ge B_4$

$$\begin{aligned} &D_{1,1}D_{2,3} - D_{1,2}D_{1,3} \\ &= \frac{1}{4}B_1^2B_2B_3(B_1 - B_2)(B_1 - B_3) \\ &\quad \cdot (-1 + 16B_1 - 4(B_1 - B_2) - 4(B_1 - B_3) - 16(B_1 - B_2)(B_1 - B_3)) \\ &\ge \frac{1}{4}B_1^2B_2B_3(B_1 - B_2)(B_1 - B_3)(-1 + 16B_1 - 8(B_1 - B_4) - 16(B_1 - B_4)^2) \\ &= \frac{B_2B_3(B_1 - B_2)(B_1 - B_3)}{B_4^2(B_1 - B_4)^2}(D_{1,1}D_{4,4} - D_{1,4}^2). \end{aligned}$$

(iv): When $A_1 = A_2$ or $X = 0$, the claim is obvious. Assume that $A_1 < A_2$ and $X > 0$. Using (2.31) with $\gamma = B_1$, we can see that $D_{1,2} \ge D_{2,2}$ if and only if $(B_1 + 2B_2)(B_1 - B_2) - 4B_1(B_1 - B_2)^2 \ge 0$. Since $B_1 - B_2 > 0$, this is equivalent to $B_1 + 2B_2 - 4B_1(B_1 - B_2) \ge 0$, or $B_1 - B_2 \le \frac{3B_1}{2(2B_1+1)}$.

(v): The proof is parallel to the proof of (iv).

(vi): By the assumption and (iv) $B_1 - B_M \le \frac{3B_1}{2(2B_1+1)}$, which implies that $B_1 - B_m \le \frac{3B_1}{2(2B_1+1)}$ for any $m \in \{1, 2, \cdots, M\}$. Again by (iv) $D_{1,m} \ge D_{m,m} \ge D_{M,M}$ for any $m \in \{1, 2, \cdots, M\}$.

(vii): The claim is trivial when $A_1 = A_2$ or $X = 0$. Let us assume that $A_1 < A_2$ and $X > 0$. By Lemma 2.11 (i)

(2.34)

$$\begin{aligned} &\frac{1}{2} - (B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}}) \ge \frac{1}{2} - (B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}})|_{X=\alpha(A_1,A_2)} \\ &= \frac{3((3+\sqrt{5})/2 - (A_1/A_2)^{\frac{1}{3}})((A_1/A_2)^{\frac{1}{3}} - (3-\sqrt{5})/2)}{2\sqrt{1 + (A_1/A_2)^{\frac{1}{3}} + (A_1/A_2)^{\frac{2}{3}}}\left(\sqrt{1 + (A_1/A_2)^{\frac{1}{3}} + (A_1/A_2)^{\frac{2}{3}}} + 2(1 - (A_1/A_2)^{\frac{1}{3}})\right)} \\ &\ge c\left(\left(\frac{A_1}{A_2}\right)^{\frac{1}{3}} - \frac{3-\sqrt{5}}{2}\right) \\ &= c\frac{A_1/A_2 - ((3-\sqrt{5})/2)^3}{(A_1/A_2)^{\frac{2}{3}} + ((3-\sqrt{5})/2)(A_1/A_2)^{\frac{1}{3}} + ((3-\sqrt{5})/2)^2} \ge c\left(\frac{A_1}{A_2} - 9 + 4\sqrt{5}\right). \end{aligned}$$

On the other hand, by (v) $2(2B_1 + 1)(B_1 - B_2) \ge 3B_1$, which implies that $4B_1^2 \ge 4B_1^2 - 4B_1B_2 - 2B_2 \ge B_1$. Thus $B_1 \ge \frac{1}{4}$. Since the function $x \mapsto \frac{x}{2x+1} : \mathbb{R}_{\ge 0} \to \mathbb{R}$ is increasing,

$$B_1 - B_2 \ge \frac{3B_1}{2(2B_1 + 1)} \ge \left.\frac{3x}{2(2x + 1)}\right|_{x=\frac{1}{4}} = \frac{1}{4}.$$

By combining this inequality with Lemma 2.11 (i)

$$\frac{1}{4} \le (B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}})(B_1^{\frac{1}{2}} + B_2^{\frac{1}{2}}) \le \frac{1-(A_1/A_2)^{\frac{1}{3}}}{\sqrt{1+(A_1/A_2)^{\frac{1}{3}}+(A_1/A_2)^{\frac{2}{3}}}}(B_1^{\frac{1}{2}} + B_2^{\frac{1}{2}}).$$

Therefore

(2.35)

$$\begin{aligned} B_1^{\frac{1}{2}} + B_2^{\frac{1}{2}} - \frac{1}{2} &\ge \frac{\sqrt{1+(A_1/A_2)^{\frac{1}{3}}+(A_1/A_2)^{\frac{2}{3}}}}{4(1-(A_1/A_2)^{\frac{1}{3}})} - \frac{1}{2} \\ &= \frac{3((3+\sqrt{5})/2-(A_1/A_2)^{\frac{1}{3}})((A_1/A_2)^{\frac{1}{3}}-(3-\sqrt{5})/2)}{4(1-(A_1/A_2)^{\frac{1}{3}})\big(\sqrt{1+(A_1/A_2)^{\frac{1}{3}}+(A_1/A_2)^{\frac{2}{3}}}+2(1-(A_1/A_2)^{\frac{1}{3}})\big)} \\ &\ge c\left(\left(\frac{A_1}{A_2}\right)^{\frac{1}{3}} - \frac{3-\sqrt{5}}{2}\right) \ge c\left(\frac{A_1}{A_2} - 9 + 4\sqrt{5}\right). \end{aligned}$$

By combining (2.34), (2.35) with the equality derived in (ii) we obtain the claimed inequality. □

We also need the following basic lemma.

Lemma 2.13. *Let* $M \in \mathbb{N}_{\ge 2}$, $\mathbf{a} = (a_j)_{j=1}^M$, $\mathbf{b} = (b_j)_{j=1}^M \in \mathbb{R}^M$, $a_1 \neq 0$, $b_1 = 0$, $b_j > 0$ $(j = 2, \cdots, M)$. *Then for any* $\mathbf{x} = (x_j)_{j=1}^M \in \mathbb{R}_{\ge 0}^M$ *satisfying* $\sum_{j=1}^M x_j = 1$

$$\langle \mathbf{a}, \mathbf{x}\rangle_{\mathbb{R}^M}^2 + \langle \mathbf{b}, \mathbf{x}\rangle_{\mathbb{R}^M}^2 \ge \min_{j\in\{2,3,\cdots,M\}} \frac{a_1^2 b_j^2}{(a_j - a_1)^2 + b_j^2}.$$

Proof. Let us define the function $f : \mathbb{R}_{\ge 0}^{M-1} \to \mathbb{R}$ by

$$f(x_2, \cdots, x_M) := \left(a_1 + \sum_{j=2}^M (a_j - a_1)x_j\right)^2 + \left(\sum_{j=2}^M b_j x_j\right)^2.$$

The function f attains its global minimum. Indeed $f(\mathbf{0}) = a_1^2$, $f(\mathbf{x}) \ge a_1^2$ for any $\mathbf{x} = (x_j)_{j=2}^M \in \mathbb{R}_{\ge 0}^{M-1}$ satisfying $\sum_{j=2}^M b_j x_j \ge |a_1|$. Thus a global minimum point of $f(\cdot)$ exists in the compact set

$$\left\{ (x_j)_{j=2}^M \in \mathbb{R}_{\ge 0}^{M-1} \;\middle|\; \sum_{j=2}^M b_j x_j \le |a_1| \right\}.$$

Observe that for any $\mathbf{x} = (x_j)_{j=1}^M \in \mathbb{R}_{\ge 0}^M$ satisfying $\sum_{j=1}^M x_j = 1$

$$\langle \mathbf{a}, \mathbf{x}\rangle_{\mathbb{R}^M}^2 + \langle \mathbf{b}, \mathbf{x}\rangle_{\mathbb{R}^M}^2 = f(x_2, \cdots, x_M).$$

Thus it suffices to prove that for any $M \in \mathbb{N}_{\ge 2}$

(Ineq(M))

$$\min_{\mathbf{x}\in\mathbb{R}_{\ge 0}^{M-1}} f(\mathbf{x}) \ge \min_{j\in\{2,3,\cdots,M\}} \frac{a_1^2 b_j^2}{(a_j - a_1)^2 + b_j^2},$$

$\forall \mathbf{a} = (a_j)_{j=1}^M,\ \mathbf{b} = (b_j)_{j=1}^M \in \mathbb{R}^M$ satisfying $a_1 \neq 0,\ b_1 = 0,\ b_j > 0\ (j = 2, \cdots, M)$.

Let us prove (Ineq(M)) by induction with M. If $M = 2$,

$$\begin{aligned} f(x_2) &= ((a_2 - a_1)^2 + b_2^2)\left(x_2 + \frac{a_1(a_2 - a_1)}{(a_2 - a_1)^2 + b_2^2}\right)^2 + \frac{a_1^2 b_2^2}{(a_2 - a_1)^2 + b_2^2} \\ &\geq \frac{a_1^2 b_2^2}{(a_2 - a_1)^2 + b_2^2} \end{aligned}$$

for any $x_2 \in \mathbb{R}_{\geq 0}$. Thus (Ineq(2)) holds. Assume that $M \geq 3$ and (Ineq($M-1$)) holds. Let us consider the case that

$$\frac{a_j - a_1}{b_j} = \frac{a_M - a_1}{b_M},\ \forall j \in \{2, 3, \cdots, M-1\}.$$

It follows that

$$\begin{aligned} f((x_j)_{j=2}^M) &= \left(a_1 + \frac{a_M - a_1}{b_M}\sum_{j=2}^M b_j x_j\right)^2 + \left(\sum_{j=2}^M b_j x_j\right)^2 \\ &\geq \min_{x \in \mathbb{R}_{\geq 0}} ((a_1 + (a_M - a_1)x)^2 + (b_M x)^2) \geq \frac{a_1^2 b_M^2}{(a_M - a_1)^2 + b_M^2}. \end{aligned}$$

In the last inequality we used (Ineq(2)). Thus the claimed inequality holds in this case. Next we consider the case that there exists $l \in \{2, 3, \cdots, M-1\}$ such that $\frac{a_l - a_1}{b_l} \neq \frac{a_M - a_1}{b_M}$. Suppose that $f(\cdot)$ attains its minimum at $(\hat{x}_j)_{j=2}^M \in \mathbb{R}_{>0}^{M-1}$. Then for $m \in \{l, M\}$

$$\frac{1}{b_m}\frac{\partial f}{\partial x_m}((\hat{x}_j)_{j=2}^M) = 2\frac{a_m - a_1}{b_m}\left(a_1 + \sum_{j=2}^M (a_j - a_1)\hat{x}_j\right) + 2\sum_{j=2}^M b_j \hat{x}_j = 0.$$

Since $\frac{a_l - a_1}{b_l} \neq \frac{a_M - a_1}{b_M}$, $\sum_{j=2}^M b_j \hat{x}_j = 0$, which is impossible. Thus $f(\cdot)$ attains its global minimum in $\mathbb{R}_{\geq 0}^{M-1} \backslash \mathbb{R}_{>0}^{M-1}$. Using the induction hypothesis,

$$\begin{aligned} &\min_{(x_j)_{j=2}^M \in \mathbb{R}_{\geq 0}^{M-1}} f((x_j)_{j=2}^M) = \min_{(x_j)_{j=2}^M \in \mathbb{R}_{\geq 0}^{M-1} \backslash \mathbb{R}_{>0}^{M-1}} f((x_j)_{j=2}^M) \\ &= \min_{j \in \{2, \cdots, M\}} \min_{(x_2, \cdots, x_{j-1}, x_{j+1}, \cdots, x_M) \in \mathbb{R}_{\geq 0}^{M-2}} f(x_2, \cdots, x_{j-1}, 0, x_{j+1}, \cdots, x_M) \\ &\geq \min_{j \in \{2, \cdots, M\}} \min_{k \in \{2, 3, \cdots, M\} \backslash \{j\}} \frac{a_1^2 b_k^2}{(a_k - a_1)^2 + b_k^2} = \min_{j \in \{2, \cdots, M\}} \frac{a_1^2 b_j^2}{(a_j - a_1)^2 + b_j^2}. \end{aligned}$$

Thus the claimed inequality holds in this case, too. Thus (Ineq(M)) holds. By induction (Ineq(M)) holds for any $M \in \mathbb{N}_{\geq 2}$, which completes the proof. □

With these tools we can find a lower bound on the right-hand side of (2.32).

Lemma 2.14. *Assume that* $\frac{e_{min}}{e_{max}} \geq \sqrt{9 - 4\sqrt{5}}$. *Then there exists* $c \in \mathbb{R}_{>0}$ *independent of any parameter such that*

$$\langle (s_j)_{j=1}^M, (D_{i,j})_{1 \leq i,j \leq M} (s_j)_{j=1}^M \rangle_{\mathbb{R}^M} \geq c B_M^3 \left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2$$

for any $M \in \mathbb{N}$, $(s_j)_{j=1}^M \in \mathbb{S}(M)$, $(A_j)_{j=1}^M \in \mathbb{A}(M)$ *and* $X \in \mathbb{R}_{\geq 0}$.

Proof. For $M \in \mathbb{N}$, $c \in \mathbb{R}_{>0}$ we set the proposition

$$\text{(Prop}(M,c)) \qquad \langle (s_j)_{j=1}^M, (D_{i,j})_{1\le i,j\le M}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M} \ge cB_M^3\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2,$$
$$\forall (s_j)_{j=1}^M \in \mathbb{S}(M),\ (A_j)_{j=1}^M \in \mathbb{A}(M),\ X \in \mathbb{R}_{\ge 0}.$$

When $M = 1$,

$$\langle (s_j)_{j=1}^M, (D_{i,j})_{1\le i,j\le M}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M} = D_{1,1} = B_1^3 \ge B_M^3\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2.$$

Thus (Prop$(1,c)$) holds for any $c \in (0,1]$. Assume that $M \ge 2$, $c_0 \in (0,1]$ and (Prop$(M-1,c_0)$) holds. We temporarily assume that $\frac{A_1}{A_M} > 9 - 4\sqrt{5}$ and $X > 0$. First let us consider the case that $D_{1,M} \ge D_{M,M}$. Lemma 2.12 (vi) ensures that $D_{1,m} \ge D_{M,M}$ for any $m \in \{1,\cdots,M\}$. By using this inequality and the induction hypothesis

$$\begin{aligned}
&\langle (s_j)_{j=1}^M, (D_{i,j})_{1\le i,j\le M}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M}\\
&\ge \langle (s_j)_{j=1}^M, \begin{pmatrix} D_{M,M} & \cdots & D_{M,M} \\ \vdots & (D_{i,j})_{2\le i,j\le M} & \\ D_{M,M} & & \end{pmatrix}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M}\\
&= D_{M,M}\left(s_1^2 + 2\sum_{j=2}^M s_1 s_j\right) + \langle (s_j)_{j=2}^M, (D_{i,j})_{2\le i,j\le M}(s_j)_{j=2}^M\rangle_{\mathbb{R}^{M-1}}\\
&= D_{M,M}\left(1 - \left(\sum_{j=2}^M s_j\right)^2\right)\\
&\quad + \left(\sum_{j=2}^M s_j\right)^2 \langle \frac{1}{\sum_{j=2}^M s_j}(s_j)_{j=2}^M, (D_{i,j})_{2\le i,j\le M}\frac{1}{\sum_{j=2}^M s_j}(s_j)_{j=2}^M\rangle_{\mathbb{R}^{M-1}}\\
&\ge B_M^3\left(1 - \left(\sum_{j=2}^M s_j\right)^2\right) + c_0 B_M^3\left(\frac{A_2}{A_M} - 9 + 4\sqrt{5}\right)^2\left(\sum_{j=2}^M s_j\right)^2\\
&\ge c_0 B_M^3\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2.
\end{aligned}$$

Next let us consider the case that $D_{1,M} < D_{M,M}$. In the following c_1 denotes a generic positive constant independent of any parameter. By using Lemma 2.12 (iii), (vii), Lemma 2.13 and Lemma 2.12 (i) in this order

$$\begin{aligned}
&\langle (s_j)_{j=1}^M, (D_{i,j})_{1\le i,j\le M}(s_j)_{j=1}^M\rangle_{\mathbb{R}^M}\\
&= D_{1,1}s_1^2 + 2\sum_{j=2}^M D_{1,j}s_j s_1 + \langle (s_j)_{j=2}^M, (D_{i,j})_{2\le i,j\le M}(s_j)_{j=2}^M\rangle_{\mathbb{R}^{M-1}}\\
&= D_{1,1}s_1^2 + 2\sum_{j=2}^M D_{1,j}s_j s_1 + \sum_{j=2}^M D_{j,j}s_j^2 + 2\sum_{l=2}^M\sum_{m=2}^M 1_{l<m}D_{l,m}s_l s_m\\
&= \frac{1}{D_{1,1}}\Bigg(\left(\sum_{j=1}^M D_{1,j}s_j\right)^2 + \sum_{j=2}^M (D_{1,1}D_{j,j} - D_{1,j}^2)s_j^2
\end{aligned}$$

$$
\begin{aligned}
&\qquad + 2\sum_{l=2}^{M}\sum_{m=2}^{M} 1_{l<m}(D_{1,1}D_{l,m} - D_{1,l}D_{1,m})s_l s_m\Bigg) \\
&\geq \frac{1}{D_{1,1}}\Bigg(\left(\sum_{j=1}^{M} D_{1,j}s_j\right)^2 + \sum_{j=2}^{M}\frac{B_j^2(B_1-B_j)^2}{B_M^2(B_1-B_M)^2}(D_{1,1}D_{M,M} - D_{1,M}^2)s_j^2 \\
&\qquad + 2\sum_{l=2}^{M}\sum_{m=2}^{M} 1_{l<m}\frac{B_l B_m(B_1-B_l)(B_1-B_m)}{B_M^2(B_1-B_M)^2}(D_{1,1}D_{M,M} - D_{1,M}^2)s_l s_m\Bigg) \\
&\geq \frac{c_1}{D_{1,1}}\Bigg(\left(\sum_{j=1}^{M} D_{1,j}s_j\right)^2 + \sum_{j=2}^{M} B_1^2 B_j^2 (B_1-B_j)^2\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2 s_j^2 \\
&\qquad + 2\sum_{l=2}^{M}\sum_{m=2}^{M} 1_{l<m}B_1^2 B_l B_m (B_1-B_l)(B_1-B_m)\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2 s_l s_m\Bigg) \\
&= \frac{c_1}{D_{1,1}}\Bigg(\langle (D_{1,j})_{j=1}^{M}, (s_j)_{j=1}^{M}\rangle_{\mathbb{R}^M}^2 \\
&\qquad + \langle \left(B_1 B_j (B_1-B_j)\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)\right)_{j=2}^{M}, (s_j)_{j=2}^{M}\rangle_{\mathbb{R}^{M-1}}^2\Bigg) \\
&\geq \frac{c_1}{D_{1,1}}\min_{j\in\{2,\cdots,M\}}\frac{D_{1,1}^2 B_1^2 B_j^2 (B_1-B_j)^2 (A_1/A_M - 9 + 4\sqrt{5})^2}{(D_{1,1}-D_{1,j})^2 + B_1^2 B_j^2 (B_1-B_j)^2 (A_1/A_M - 9 + 4\sqrt{5})^2} \\
&\geq c_1 \min_{j\in\{2,\cdots,M\}}\frac{D_{1,1} B_1^2 B_j^2 (B_1-B_j)^2 (A_1/A_M - 9 + 4\sqrt{5})^2}{B_1^4 (B_1-B_j)^2 + B_1^2 B_j^2 (B_1-B_j)^2 (A_1/A_M - 9 + 4\sqrt{5})^2} \\
&\geq c_1 B_M^3\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2.
\end{aligned}
$$

Here we remark that we used the assumptions $\frac{A_1}{A_M} > 9 - 4\sqrt{5}$ and $X > 0$ to apply Lemma 2.12 (iii), Lemma 2.13. Thus

$$
\langle (s_j)_{j=1}^{M}, (D_{i,j})_{1\leq i,j\leq M}(s_j)_{j=1}^{M}\rangle_{\mathbb{R}^M} \geq \min\{c_0, c_1\}B_M^3\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2
$$

for any $(s_j)_{j=1}^{M} \in \mathbb{S}(M)$, $(A_j)_{j=1}^{M} \in \mathbb{A}(M)$ satisfying $\frac{A_1}{A_M} > 9 - 4\sqrt{5}$ and $X \in \mathbb{R}_{>0}$. Since the both sides of the above inequality are continuous with A_1, A_M, X, (Prop(M, $\min\{c_0, c_1\}$)) holds by taking the limit. It follows that if (Prop($M - 1, \min\{1, c_1\}$)) holds, then (Prop($M, \min\{1, c_1\}$)) holds. By induction with M (Prop($M, \min\{1, c_1\}$)) holds for any $M \in \mathbb{N}$. The proof is complete. □

We are ready to prove Lemma 2.9.

Proof of Lemma 2.9. By Lemma 2.10 and Lemma 2.14

$$
\begin{aligned}
&\frac{C_1}{C_2^3}(4C_2^2 + C_1C_2 - 4C_1C_3) \geq c\frac{C_1}{C_2^3}B_M^3\left(\frac{A_1}{A_M} - 9 + 4\sqrt{5}\right)^2 \\
&\geq c\frac{B_M^4}{B_1^6}\left(\left(\frac{e_{min}}{e_{max}}\right)^2 - 9 + 4\sqrt{5}\right)^2
\end{aligned}
$$

$$\geq c \inf_{X \in \mathbb{R}_{\geq 0}} \left(\frac{1 + A_1 X}{1 + A_M X} \right)^6 \left(\left(\frac{e_{min}}{e_{max}} \right)^2 - 9 + 4\sqrt{5} \right)^2$$

$$= c \left(\frac{A_1}{A_M} \right)^6 \left(\left(\frac{e_{min}}{e_{max}} \right)^2 - 9 + 4\sqrt{5} \right)^2 \geq c(9 - 4\sqrt{5})^6 \left(\left(\frac{e_{min}}{e_{max}} \right)^2 - 9 + 4\sqrt{5} \right)^2.$$

□

Here we can prove the positivity of $\frac{d^2\tau}{d\beta^2}(\beta)$ for small β as follows.

Lemma 2.15. *Assume that* $\frac{e_{min}}{e_{max}} > \sqrt{9 - 4\sqrt{5}}$. *Let* $M(e_{min}, e_{max}) \in \mathbb{R}_{>0}$ *be that introduced in Lemma 2.2. Then there exist* $c \in \mathbb{R}_{>0}$ *independent of any parameter and* $U_0 \in (0, \frac{e_{min}}{\sinh(2)b}]$ *such that for any* $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$, $\beta \in (0, \beta_c)$ *satisfying* $\beta \leq M(e_{min}, e_{max})\sqrt{1 + y(\beta)}$

$$\frac{d^2\tau}{d\beta^2}(\beta) \geq c \frac{\sqrt{1 + y(\beta)}}{\beta^2} \left(\left(\frac{e_{min}}{e_{max}} \right)^2 - 9 + 4\sqrt{5} \right)^2.$$

Proof. Combination of Lemma 2.8, (2.28) and Lemma 2.9 yields the result. Here we remark that the condition $\frac{e_{min}}{e_{max}} > \sqrt{9 - 4\sqrt{5}}$ is necessary to ensure that (2.26) holds. □

Lemma 2.5 and Lemma 2.15 imply the following.

Corollary 2.16. *Assume that* $\frac{e_{min}}{e_{max}} > \sqrt{9 - 4\sqrt{5}}$. *Then there exists* $U_0 \in (0, \frac{e_{min}}{\sinh(2)b}]$ *such that for any* $U \in [-U_0, 0)$ *and* $E \in \mathcal{E}(e_{min}, e_{max})$

$$\lim_{\beta \searrow 0} \frac{d^2\tau}{d\beta^2}(\beta) = +\infty.$$

Finally we achieve the goal of this section.

Proof of Proposition 1.6. The claim follows from Lemma 2.2, Corollary 2.3, Lemma 2.15 and Corollary 2.16. □

3 Non-convexity of the phase boundary: non-critical case

In this section we prove Proposition 1.7. Our proof is based on the relation (2.23) and Lemma 2.7. It is essential to find $E \in \mathcal{E}(e_{min}, e_{max})$ such that the function $\tilde{W}_E(\cdot)$ takes a negative value. We begin by constructing basic properties which we need to analyze the function $\tilde{W}_E(\cdot)$. Let us recall the notations (2.29), (2.30), (2.33). Here we add more properties of $D_{i,j}$.

Lemma 3.1. *Let* A_1, $A_2 \in \mathbb{R}_{>0}$ *satisfy* $A_1 \leq A_2$.

(i) Assume that $\frac{A_1}{A_2} \leq 9 - 4\sqrt{5}$. *Then* $D_{1,2}|_{X=\alpha(A_1,A_2)} < 0$.

(ii) Assume that $\frac{A_1}{A_2} < 9 - 4\sqrt{5}$. *Then*

$$(D_{1,1}D_{2,2} - D_{1,2}^2)|_{X=\alpha(A_1,A_2)} < 0.$$

(iii) Assume that $\frac{A_1}{A_2} < 9 - 4\sqrt{5}$. *Set*

$$s_1 := \frac{|D_{1,2}|}{D_{1,1} + |D_{1,2}|}\bigg|_{X=\alpha(A_1,A_2)}, \ s_2 := \frac{D_{1,1}}{D_{1,1} + |D_{1,2}|}\bigg|_{X=\alpha(A_1,A_2)}.$$

Then s_1, $s_2 \in (0,1)$, $s_1 + s_2 = 1$ *and*

$$\langle (s_j)_{j=1}^2, (D_{i,j})_{1\le i,j\le 2}|_{X=\alpha(A_1,A_2)}(s_j)_{j=1}^2\rangle_{\mathbb{R}^2} < 0.$$

Proof. (i): By the assumption Lemma 2.11 implies that

$$(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}})|_{X=\alpha(A_1,A_2)} = \max_{X\in\mathbb{R}_{\ge 0}}(B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}}) \ge \frac{1}{2}.$$

We can deduce from (2.31) for $D_{1,2}$, $\gamma = B_2$ that $D_{1,2} < 0$ if and only if $B_1 > B_2 + \frac{1}{8}(1 + \sqrt{1 + 32B_2})$. If $B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}} \ge \frac{1}{2}$,

$$B_1 \ge B_2 + B_2^{\frac{1}{2}} + \frac{1}{4} > B_2 + \frac{1}{8}(1 + \sqrt{1 + 32B_2}),$$

and thus the claim holds.

(ii): By the assumption and Lemma 2.11 $\frac{1}{2} - (B_1^{\frac{1}{2}} - B_2^{\frac{1}{2}})|_{X=\alpha(A_1,A_2)} < 0$, and thus $B_1^{\frac{1}{2}}|_{X=\alpha(A_1,A_2)} > \frac{1}{2}$. By combining these inequalities with Lemma 2.12 (ii) we can derive the claimed inequality.

(iii): By (i) s_1, $s_2 \in (0,1)$ and $s_1 + s_2 = 1$. Observe that

$$\begin{aligned}(3.1)\quad &\langle (s_j)_{j=1}^2, (D_{i,j})_{1\le i,j\le 2}|_{X=\alpha(A_1,A_2)}(s_j)_{j=1}^2\rangle_{\mathbb{R}^2} \\ &= \frac{1}{D_{1,1}}(D_{1,1}s_1 + D_{1,2}s_2)^2\bigg|_{X=\alpha(A_1,A_2)} + \frac{s_2^2}{D_{1,1}}(D_{1,1}D_{2,2} - D_{1,2}^2)\bigg|_{X=\alpha(A_1,A_2)}.\end{aligned}$$

By (i) and the definition of s_1, s_2 the 1st term of the right-hand side of (3.1) vanishes. By (ii) the 2nd term of the right-hand side of (3.1) is negative, which concludes the proof. □

We will use the next lemma in the proof of Proposition 1.7.

Lemma 3.2. *Set*

$$x_0 := \sqrt{2\frac{e_{min}^{\frac{2}{3}} + e_{max}^{\frac{2}{3}}}{e_{min}^{\frac{4}{3}}e_{max}^{\frac{4}{3}}}}. \tag{3.2}$$

For any $E \in \mathcal{E}(e_{min}, e_{max})$ *there exists* $U_0 \in (0, \frac{2e_{min}}{b})$ *such that the following statement holds. For any* $U \in [-U_0, 0)$ *there exists* $Y \in (-1, 0)$ *such that* $\sqrt{1+Y}x_0 \in (0, \beta_c)$ *and* $y(\sqrt{1+Y}x_0) = Y$, *where* $y(\beta) := \cos(\frac{\tau(\beta)}{2})$ *for* $\beta \in (0, \beta_c)$.

Proof. According to Lemma 1.1,

$$\beta_c \le \frac{2}{e_{min}}\tanh^{-1}\left(\frac{b|U|}{2e_{min}}\right), \ \forall U \in \left(-\frac{2e_{min}}{b}, 0\right).$$

Thus there exists $U_0 \in (0, \frac{2e_{min}}{b})$ such that $\beta_c < x_0$ for any $U \in [-U_0, 0)$. Fix $U \in [-U_0, 0)$. Since $\lim_{\beta\nearrow\beta_c}\sqrt{1 + y(\beta)}/\beta = 0$ by Lemma 1.2 (ii), there exists

$\eta \in \mathbb{R}_{>0}$ such that $\sqrt{1+y(\beta)} \le \frac{\beta}{x_0}$ for any $\beta \in [\beta_c - \eta, \beta_c)$. Since $\beta_c < x_0$, there exists $\tilde{Y} \in (-1, 0)$ such that $\sqrt{1+\tilde{Y}}x_0 \in [\beta_c - \eta, \beta_c)$. It follows that

$$\sqrt{1 + y\big(\sqrt{1+\tilde{Y}}x_0\big)} \le \frac{\sqrt{1+\tilde{Y}}x_0}{x_0} = \sqrt{1+\tilde{Y}},$$

or

$$y\big(\sqrt{1+\tilde{Y}}x_0\big) \le \tilde{Y}. \tag{3.3}$$

On the other hand, by Lemma 2.5 $\lim_{\beta \searrow 0} \beta^2/(1+y(\beta)) = 0$. Thus $\lim_{Y \searrow -1}(1+Y)/(1+y(\sqrt{1+Y}x_0)) = 0$. Therefore there exists $\hat{Y} \in (-1, \tilde{Y})$ such that $1+\hat{Y} < 1 + y(\sqrt{1+\hat{Y}}x_0)$ or

$$\hat{Y} < y\big(\sqrt{1+\hat{Y}}x_0\big). \tag{3.4}$$

By (3.3), (3.4) and the continuity of $y(\cdot)$ there exists $Y \in (\hat{Y}, \tilde{Y}]$ such that $\sqrt{1+Y}x_0 \in (0, \beta_c)$ and $Y = y(\sqrt{1+Y}x_0)$. □

We need to construct $E \in \mathcal{E}(e_{min}, e_{max})$ for which $\tau(\cdot)$ is non-convex. As mentioned at the beginning of the section, we must show that $\tilde{W}_E(\cdot)$ takes a negative value. We achieve this as follows. First we find a matrix-valued discontinuous function $E_\infty : \Gamma_\infty^* \to \mathrm{Mat}(b, \mathbb{C})$ such that $\tilde{W}_{E_\infty}(\cdot)$ takes a negative value. Then we approximate E_∞ by some $E \in \mathcal{E}(e_{min}, e_{max})$ so that $\tilde{W}_E(\cdot)$ has the desired property.

Remark 3.3. One question we expect here is why we do not try to establish the same theorem without assuming the smoothness of one-particle Hamiltonian matrix E if such an example is found in a non-smooth class. This is because we cannot justify the derivation of our gap equation if we allow one-particle Hamiltonian matrix to be discontinuous. Polynomial decay property of the free propagator with the spatial variables, which is guaranteed by smoothness of one-particle Hamiltonian matrix with the momentum variables, is essential in the derivation of the infinite-volume limit [13, Theorem 1.3] via multi-scale analysis. However, it is possible to reduce the smoothness condition to some continuous differentiability condition to derive the infinite-volume limit as claimed in [13, Theorem 1.3]. We assume the smoothness condition throughout for simplicity.

In the following until the proof of Proposition 1.7 we assume that $\frac{e_{min}}{e_{max}} \le \sqrt{9 - 4\sqrt{5}}$. Similarly to the definition in Lemma 3.1 (iii), we set

$$s_1 := \frac{|D_{1,2}|}{D_{1,1} + |D_{1,2}|}\Bigg|_{\substack{A_1 = e_{min}^2, A_2 = e_{max}^2, \\ X = \alpha(A_1, A_2)}}, \quad s_2 := 1 - s_1. \tag{3.5}$$

By Lemma 3.1 (i) $s_1, s_2 \in (0, 1)$. Let us define the function $\Phi_\infty : \mathbb{R}^d \to \mathbb{R}$ by

$$\Phi_\infty(x_1, \cdots, x_d) := \begin{cases} e_{max} & \text{if } |x_j - \pi| < \pi s_2^{\frac{1}{d}} \text{ for all } j \in \{1, \cdots, d\}, \\ e_{min} & \text{otherwise.} \end{cases}$$

Then we define $E_\infty : \Gamma_\infty^* \to \mathrm{Mat}(b, \mathbb{C})$ by $E_\infty(\mathbf{k}) := \Phi_\infty((\hat{\mathbf{v}}_1, \cdots, \hat{\mathbf{v}}_d)^{-1}\mathbf{k})I_b$. Observe that for any continuous function $f : \mathbb{R}\backslash\{0\} \to \mathbb{C}$

$$D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\, f(E_\infty(\mathbf{k})) = b(s_1 f(e_{min}) + s_2 f(e_{max})). \tag{3.6}$$

In the following we construct $\{E_p\}_{p\in\mathbb{R}_{>0}} \subset \mathcal{E}(e_{min}, e_{max})$ such that E_p approximates E_∞ as $p \to \infty$. Define the function $\phi_p \in C^\infty(\mathbb{R})$ ($p \in \mathbb{R}_{>0}$) by

$$\phi_p(x) := \begin{cases} \exp\left(\frac{1}{(\pi s_2^{1/d})^{-2p}((x-\pi)^2)^p - 1} + 1\right) & \text{if } |x-\pi| < \pi s_2^{\frac{1}{d}}, \\ 0 & \text{otherwise.} \end{cases}$$

Then we define $\Phi_p \in C^\infty(\mathbb{R}^d)$ ($p \in \mathbb{R}_{>0}$) by

$$\Phi_p(x_1, \cdots, x_d) := (e_{max} - e_{min}) \prod_{j=1}^{d} \phi_p(x_j) + e_{min}.$$

Then we define $\hat{E}_p : \Gamma_\infty^* \to \mathrm{Mat}(b, \mathbb{C})$ by $\hat{E}_p(\mathbf{k}) := \Phi_p((\hat{\mathbf{v}}_1, \cdots, \hat{\mathbf{v}}_d)^{-1}\mathbf{k}) I_b$. Finally we define $E_p : \mathbb{R}^d \to \mathrm{Mat}(b, \mathbb{C})$ ($p \in \mathbb{R}_{>0}$) by $E_p(\mathbf{k}) := \hat{E}_p(\hat{\mathbf{k}})$, where $\hat{\mathbf{k}} \in \{(\hat{\mathbf{v}}_1, \cdots, \hat{\mathbf{v}}_d)\tilde{\mathbf{k}} \mid \tilde{\mathbf{k}} \in [0, 2\pi)^d\}$ and $\mathbf{k} = \hat{\mathbf{k}} + \sum_{j=1}^d 2\pi m_j \hat{\mathbf{v}}_j$ for some $(m_j)_{j=1}^d \in \mathbb{Z}^d$.

Lemma 3.4. *The following statements hold true.*

(i) $\{E_p\}_{p\in\mathbb{R}_{>0}} \subset \mathcal{E}(e_{min}, e_{max})$.

(ii) For any continuous function $f : \mathbb{R}\backslash\{0\} \to \mathbb{C}$

$$\lim_{p\to\infty} D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\, f(E_p(\mathbf{k})) = D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\, f(E_\infty(\mathbf{k})).$$

Remark 3.5. We have already proved similar lemmas [13, Lemma A.1], [14, Lemma 2.9]. Though the previously constructed families of $\mathcal{E}(e_{min}, e_{max})$ are different from $\{E_p\}_{p\in\mathbb{R}_{>0}}$, these lemmas are essentially applicable to prove Proposition 1.7 and Proposition 1.8. We present Lemma 3.4 in the belief that the construction of $\{E_p\}_{p\in\mathbb{R}_{>0}}$ is simpler and more suited for our present purposes. Also, containing all the necessary lemmas must be convenient for the readers.

Proof of Lemma 3.4. (i): We only check the property (1.9), as the other properties apparently hold. Take any $\mathbf{k} \in \mathbb{R}^d$. There exist $(\tilde{k}_j)_{j=1}^d \in [0, 2\pi)^d$, $(m_j)_{j=1}^d \in \mathbb{Z}^d$ such that $\mathbf{k} = \sum_{j=1}^d \tilde{k}_j \hat{\mathbf{v}}_j + \sum_{j=1}^d 2\pi m_j \hat{\mathbf{v}}_j$. Observe that

$$\begin{aligned}\overline{E_p(-\mathbf{k})} &= E_p\left(\sum_{j=1}^d (2\pi - \tilde{k}_j)\hat{\mathbf{v}}_j\right) = \Phi_p(2\pi - \tilde{k}_1, \cdots, 2\pi - \tilde{k}_d) I_b = \Phi_p(\tilde{k}_1, \cdots, \tilde{k}_d) I_b \\ &= E_p(\mathbf{k}).\end{aligned}$$

Here we used that $\phi_p(2\pi - k) = \phi_p(k)$ for any $k \in \mathbb{R}$. Therefore (1.9) is satisfied.

(ii): Let $f : \mathbb{R}\backslash\{0\} \to \mathbb{C}$ be a continuous function. For any $\mathbf{k} \in \Gamma_\infty^*$ there exists $(\tilde{k}_j)_{j=1}^d \in [0, 2\pi]^d$ such that $\mathbf{k} = \sum_{j=1}^d \tilde{k}_j \hat{\mathbf{v}}_j$. Since $\lim_{p\to\infty} \Phi_p(\tilde{k}_1, \cdots, \tilde{k}_d) = \Phi_\infty(\tilde{k}_1, \cdots, \tilde{k}_d)$,

$$\begin{aligned}\lim_{p\to\infty} \mathrm{Tr}\, f(E_p(\mathbf{k})) &= b \lim_{p\to\infty} f(\Phi_p(\tilde{k}_1, \cdots, \tilde{k}_d)) = b f(\Phi_\infty(\tilde{k}_1, \cdots, \tilde{k}_d)) \\ &= \mathrm{Tr}\, f(E_\infty(\mathbf{k})).\end{aligned} \tag{3.7}$$

Also

$$|\mathrm{Tr}\, f(E_p(\mathbf{k}))| \le b \sup_{x\in[e_{min}, e_{max}]} |f(x)| \tag{3.8}$$

for any $p \in \mathbb{R}_{>0}$. By (3.7), (3.8) one can apply the dominated convergence theorem in $L^1(\Gamma_\infty^*)$ to ensure the claimed convergence. □

Here we can prove Proposition 1.7.

Proof of Proposition 1.7. Assume that $\frac{e_{min}}{e_{max}} < \sqrt{9-4\sqrt{5}}$. We define $\{E_p\}_{p\in\mathbb{R}_{>0}} \subset \mathcal{E}(e_{min}, e_{max})$, $E_\infty : \Gamma_\infty^* \to \mathrm{Mat}(b, \mathbb{C})$ as we did in front of Lemma 3.4. Though we originally defined the function $\tilde{W}_E(\cdot)$ for $E \in \mathcal{E}(e_{min}, e_{max})$, we can define $\tilde{W}_{E_\infty}(\cdot)$ by replacing E by E_∞ in (2.24). Recalling the notational rule given in front of Lemma 2.9 and (3.6), we see that with $A_1 := e_{min}^2$, $A_2 := e_{max}^2$, $M = 2$

$$\tilde{W}_{E_\infty}(x) = \frac{C_1}{\sqrt{2}C_2^3}(4C_2^2 + C_1C_2 - 4C_1C_3).$$

Moreover by Lemma 2.10

$$\tilde{W}_{E_\infty}(x) = \frac{C_1}{\sqrt{2}C_2^3}\langle (s_j)_{j=1}^2, (D_{i,j})_{1\le i,j\le 2}(s_j)_{j=1}^2\rangle_{\mathbb{R}^2}.$$

We define x_0 by (3.2). Since $X = \frac{x_0^2}{2} = \alpha(A_1, A_2)$ and $\frac{A_1}{A_2} < 9 - 4\sqrt{5}$, Lemma 3.1 (iii) guarantees that

$$\tilde{W}_{E_\infty}(x_0) < 0. \tag{3.9}$$

We can apply Lemma 3.4 (ii) to deduce from (3.9) that there exists $p \in \mathbb{R}_{>0}$ such that $\tilde{W}_{E_p}(x_0) < 0$. Moreover, by Lemma 2.7 there exists $y_0 \in (-1, 0)$ such that

$$W_{E_p}(x_0, y) < 0, \ \forall y \in (-1, y_0]. \tag{3.10}$$

By the 2nd inequality of Lemma 2.4 for E_p there exists $U_0 \in (0, \frac{2e_{min}}{b})$ such that $y(\beta) \in (-1, y_0]$ for all $U \in [-U_0, 0)$, $\beta \in (0, \beta_c)$. Lemma 3.2 ensures that by taking U_0 smaller if necessary for any $U \in [-U_0, 0)$ there exists $Y \in (-1, 0)$ such that $\sqrt{1+Y}x_0 \in (0, \beta_c)$ and $y(\sqrt{1+Y}x_0) = Y \in (-1, y_0]$. Set $\beta' := \sqrt{1+Y}x_0$. It follows that $y(\beta') \in (-1, y_0]$ and

$$W_{E_p}(x_0, Y) = W_{E_p}\left(\frac{\beta'}{\sqrt{1+Y}}, Y\right) = W_{E_p}\left(\frac{\beta'}{\sqrt{1+y(\beta')}}, y(\beta')\right).$$

Thus by (3.10)

$$W_{E_p}\left(\frac{\beta'}{\sqrt{1+y(\beta')}}, y(\beta')\right) < 0,$$

which combined with (2.23) implies that $\frac{d^2\tau}{d\beta^2}(\beta') < 0$. This concludes the proof. □

4 Non-convexity of the phase boundary: critical case

In this section we prove Proposition 1.8. We assume that $\frac{e_{min}}{e_{max}} = \sqrt{9-4\sqrt{5}}$ throughout this section. We want to show non-convexity of $\tau(\cdot)$, which is the same goal as in Section 3. However, there is an essential difference from the previous construction. In the present case by (2.28) and Lemma 2.9 $\tilde{W}_E(x)$ is non-negative for any $x \in \mathbb{R}_{\ge 0}$, $E \in \mathcal{E}(e_{min}, e_{max})$. This means that the same argument as in

Section 3 does not lead to the claimed result. Interestingly it will turn out that $W_{E_\infty}(x_0, y) < 0$ for $y \in (-1, 0)$ sufficiently close to -1. Based on this property and (2.23), we can choose $E \in \mathcal{E}(e_{min}, e_{max})$ so that $\tau(\cdot)$ is non-convex. The proof of the negativity of $W_{E_\infty}(x_0, y)$ is the most technical part in this paper. It requires exact computation of the limit

$$\lim_{y \searrow -1} \frac{\partial^j W_{E_\infty}}{\partial y^j}(x_0, y)$$

for $j = 0, 1, 2$. We will perform the computation separately in Subsection 4.2.

4.1 Proof of the proposition

Let the family $\{E_p\}_{p \in \mathbb{R}_{>0}} \subset \mathcal{E}(e_{min}, e_{max})$ and $E_\infty : \Gamma_\infty^* \to \mathrm{Mat}(b, \mathbb{C})$ be those constructed in front of Lemma 3.4. We have to prove in advance that various objects depending on E_p converge as $p \to \infty$. Let the functions F^p, $F^\infty : \mathbb{R}_{>0} \times (-1, 0) \to \mathbb{R}$ be defined by (2.1) with $E = E_p$, E_∞ respectively. The equality (3.6) ensures the well-definedness of F^∞. We define $W_{E_\infty} : \mathbb{R}_{>0} \times (-1, 0) \to \mathbb{R}$ by (2.22) with $E = E_\infty$. It is well-defined despite that $E_\infty \notin \mathcal{E}(e_{min}, e_{max})$. First we prove that W_{E_p} converges to W_{E_∞}.

Lemma 4.1. *For any closed bounded intervals $J \subset \mathbb{R}_{>0}$, $K \subset (-1, 0)$*

$$\lim_{p \to \infty} \sup_{\substack{x \in J \\ y \in K}} |W_{E_p}(x, y) - W_{E_\infty}(x, y)| = 0.$$

Proof. Let F_a^p, F_a^∞ $(a = x, y, xx, xy, yy)$ denote partial derivatives of the functions F^p, F^∞. Recalling the explicit forms (2.4), (2.5), (2.6), (2.7), (2.8), we can apply the dominated convergence theorem in $L^1(\Gamma_\infty^*)$ to prove that

$$\lim_{p \to \infty} \sup_{\substack{x \in J \\ y \in K}} |F_a^p(\sqrt{y+1}x, y) - F_a^\infty(\sqrt{y+1}x, y)| = 0$$

for $a = x$, y, xx, xy, yy, which implies the claimed convergence property. □

We can define the function $g_{E_\infty} : \mathbb{R}_{>0} \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ by (1.12) with $E = E_\infty$. For $E_p \in \mathcal{E}(e_{min}, e_{max})$ $(p \in \mathbb{R}_{>0})$ we write $\beta_c(p)$, $\tau(\beta, p)$ in place of β_c, $\tau(\beta)$ in order to indicate the dependency on the parameter p. The following lemma shows convergent properties of $\beta_c(p)$, $\tau(\beta, p)$ as $p \to \infty$.

Lemma 4.2. *Assume that $U \in (-\frac{2e_{min}}{b}, 0)$. Then the following statements hold.*

(i) There uniquely exists

$$\beta_{c,\infty} \in \left(0, \frac{2}{e_{min}} \tanh^{-1}\left(\frac{b|U|}{2e_{min}}\right)\right]$$

such that $g_{E_\infty}(\beta_{c,\infty}, 2\pi, 0) = 0$. Moreover $\lim_{p \to \infty} \beta_c(p) = \beta_{c,\infty}$.

(ii) For any $\beta \in (0, \beta_{c,\infty})$ there uniquely exists $\tau_\infty(\beta) \in (\pi, 2\pi)$ such that $g_{E_\infty}(\beta, \tau_\infty(\beta), 0) = 0$. Moreover the function $\beta \mapsto \tau_\infty(\beta) : (0, \beta_{c,\infty}) \to \mathbb{R}$ is real analytic and

$$\lim_{p \to \infty} \tau(\beta, p) = \tau_\infty(\beta), \ \forall \beta \in (0, \beta_{c,\infty}), \tag{4.1}$$

$$
\lim_{\beta \searrow 0} \frac{\beta}{\sqrt{1+\cos(\tau_\infty(\beta)/2)}} = 0, \tag{4.2}
$$

$$
\lim_{\beta \nearrow \beta_{c,\infty}} \tau_\infty(\beta) = 2\pi. \tag{4.3}
$$

Remark 4.3. By (i) for any $\beta \in (0, \beta_{c,\infty})$ there exists $p_0 \in \mathbb{R}_{>0}$ such that $\beta \in (0, \beta_c(p))$ for any $p \geq p_0$. In (ii) we consider $\lim_{p\to\infty} \tau(\beta, p)$ as $\lim_{p\to\infty, p\geq p_0} \tau(\beta, p)$.

Proof of Lemma 4.2. (i): The unique existence of $\beta_{c,\infty}$ satisfying the claimed properties except for the convergent property is proved by the same argument as the proof of Lemma 1.1. To prove the convergent property, suppose that $\limsup_{p\to\infty} \beta_c(p) > \beta_{c,\infty}$. There exists $\varepsilon \in \mathbb{R}_{>0}$ such that for any $p_1 \in \mathbb{R}_{>0}$ $\sup_{p\geq p_1} \beta_c(p) \geq \beta_{c,\infty} + \varepsilon$. Take any $p_1 \in \mathbb{R}_{>0}$. There exists $q \in [p_1, \infty)$ such that $\beta_c(q) \geq \beta_{c,\infty} + \frac{\varepsilon}{2}$. It follows that

$$
\begin{aligned}
0 = g_{E_q}(\beta_c(q), 2\pi, 0) &= -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta_c(q)}{2} E_q(\mathbf{k}))E_q(\mathbf{k})}\right) \\
&\leq -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta_{c,\infty}+\varepsilon/2}{2} E_q(\mathbf{k}))E_q(\mathbf{k})}\right) \\
&\leq -\frac{2}{|U|} + \sup_{p\geq p_1} D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta_{c,\infty}+\varepsilon/2}{2} E_p(\mathbf{k}))E_p(\mathbf{k})}\right).
\end{aligned}
$$

By Lemma 3.4 (ii)

$$
\begin{aligned}
0 &\leq -\frac{2}{|U|} + \limsup_{p\to\infty} D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta_{c,\infty}+\varepsilon/2}{2} E_p(\mathbf{k}))E_p(\mathbf{k})}\right) \\
&= -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta_{c,\infty}+\varepsilon/2}{2} E_\infty(\mathbf{k}))E_\infty(\mathbf{k})}\right) \\
&< -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr}\left(\frac{1}{\tanh(\frac{\beta_{c,\infty}}{2} E_\infty(\mathbf{k}))E_\infty(\mathbf{k})}\right) \\
&= g_{E_\infty}(\beta_{c,\infty}, 2\pi, 0) = 0,
\end{aligned}
$$

which is a contradiction. Thus $\limsup_{p\to\infty} \beta_c(p) \leq \beta_{c,\infty}$. Suppose that $\liminf_{p\to\infty} \beta_c(p) < \beta_{c,\infty}$. There exists $\varepsilon' \in \mathbb{R}_{>0}$ such that for any $p_2 \in \mathbb{R}_{>0}$ $\inf_{p\geq p_2} \beta_c(p) \leq \beta_{c,\infty} - \varepsilon'$. Take any $p_2 \in \mathbb{R}_{>0}$. There exists $q' \in [p_2, \infty)$ such that $\beta_c(q') \leq \beta_{c,\infty} - \frac{\varepsilon'}{2}$. Observe that

$$
0 = g_{E_{q'}}(\beta_c(q'), 2\pi, 0) \geq g_{E_{q'}}\left(\beta_{c,\infty} - \frac{\varepsilon'}{2}, 2\pi, 0\right) \geq \inf_{p\geq p_2} g_{E_p}\left(\beta_{c,\infty} - \frac{\varepsilon'}{2}, 2\pi, 0\right).
$$

Lemma 3.4 (ii) ensures that

$$
0 \geq \liminf_{p\to\infty} g_{E_p}\left(\beta_{c,\infty} - \frac{\varepsilon'}{2}, 2\pi, 0\right) = g_{E_\infty}\left(\beta_{c,\infty} - \frac{\varepsilon'}{2}, 2\pi, 0\right) > g_{E_\infty}(\beta_{c,\infty}, 2\pi, 0) = 0,
$$

which is again a contradiction. Therefore $\liminf_{p\to\infty} \beta_c(p) \geq \beta_{c,\infty}$. Summing up, we obtain that $\limsup_{p\to\infty} \beta_c(p) \leq \beta_{c,\infty} \leq \liminf_{p\to\infty} \beta_c(p)$, which implies the claimed convergence.

(ii): The same argument as the proof of Lemma 1.1 (iii) shows the unique existence of $\tau_\infty(\beta) \in (\pi, 2\pi)$. Since $(\beta, t) \mapsto g_{E_\infty}(\beta, t, 0) : \mathbb{R}_{>0} \times \mathbb{R} \to \mathbb{R}$ is real analytic and $\frac{\partial g_{E_\infty}}{\partial t}(\beta, \tau_\infty(\beta), 0) \neq 0$ for all $\beta \in (0, \beta_{c,\infty})$, the real analytic implicit function theorem (e.g. [15, Theorem 2.3.5]) ensures that $\tau_\infty(\cdot)$ is real analytic in $(0, \beta_{c,\infty})$. Take any $\beta \in (0, \beta_{c,\infty})$. Since $\lim_{p\to\infty} \beta_c(p) = \beta_{c,\infty}$, there exists $p_3 \in \mathbb{R}_{>0}$ such that $\beta \in (0, \beta_c(p))$ for any $p \geq p_3$. Let us set

$$y(\beta, p) := \cos\left(\frac{\tau(\beta, p)}{2}\right) \ (p \geq p_3), \ y_\infty(\beta) := \cos\left(\frac{\tau_\infty(\beta)}{2}\right)$$

for simplicity. Suppose that $\limsup_{p\to\infty} y(\beta, p) > y_\infty(\beta)$. There exists $\hat{\varepsilon} \in \mathbb{R}_{>0}$ such that $\sup_{p\geq p_4} y(\beta, p) \geq y_\infty(\beta) + \hat{\varepsilon}$ for any $p_4 \in [p_3, \infty)$. Take any $p_4 \in [p_3, \infty)$. There exists $\hat{q} \in [p_4, \infty)$ such that $y(\beta, \hat{q}) \geq y_\infty(\beta) + \frac{\hat{\varepsilon}}{2}$. It follows that

$$\begin{aligned} 0 = g_{E_{\hat{q}}}(\beta, \tau(\beta, \hat{q}), 0) &\leq -\frac{2}{|U|} + F^{\hat{q}}\left(\beta, y_\infty(\beta) + \frac{\hat{\varepsilon}}{2}\right) \\ &\leq -\frac{2}{|U|} + \sup_{p\geq p_4} F^p\left(\beta, y_\infty(\beta) + \frac{\hat{\varepsilon}}{2}\right). \end{aligned}$$

By arbitrariness of p_4 and Lemma 3.4 (ii)

$$\begin{aligned} 0 &\leq -\frac{2}{|U|} + \limsup_{p\to\infty} F^p\left(\beta, y_\infty(\beta) + \frac{\hat{\varepsilon}}{2}\right) = -\frac{2}{|U|} + F^\infty\left(\beta, y_\infty(\beta) + \frac{\hat{\varepsilon}}{2}\right) \\ &< g_{E_\infty}(\beta, \tau_\infty(\beta), 0) = 0, \end{aligned}$$

which is a contradiction. Thus $\limsup_{p\to\infty} y(\beta, p) \leq y_\infty(\beta)$. Suppose that $\liminf_{p\to\infty} y(\beta, p) < y_\infty(\beta)$. There exists $\tilde{\varepsilon} \in \mathbb{R}_{>0}$ such that $\inf_{p\geq p_5} y(\beta, p) \leq y_\infty(\beta) - \tilde{\varepsilon}$ for any $p_5 \in [p_3, \infty)$. Take any $p_5 \in [p_3, \infty)$. There exists $\tilde{q} \in [p_5, \infty)$ such that $y(\beta, \tilde{q}) \leq y_\infty(\beta) - \frac{\tilde{\varepsilon}}{2}$. Observe that

$$\begin{aligned} 0 = g_{E_{\tilde{q}}}(\beta, \tau(\beta, \tilde{q}), 0) &\geq -\frac{2}{|U|} + F^{\tilde{q}}\left(\beta, y_\infty(\beta) - \frac{\tilde{\varepsilon}}{2}\right) \\ &\geq -\frac{2}{|U|} + \inf_{p\geq p_5} F^p\left(\beta, y_\infty(\beta) - \frac{\tilde{\varepsilon}}{2}\right). \end{aligned}$$

Since p_5 is arbitrary, Lemma 3.4 (ii) ensures that

$$\begin{aligned} 0 &\geq -\frac{2}{|U|} + \liminf_{p\to\infty} F^p\left(\beta, y_\infty(\beta) - \frac{\tilde{\varepsilon}}{2}\right) = -\frac{2}{|U|} + F^\infty\left(\beta, y_\infty(\beta) - \frac{\tilde{\varepsilon}}{2}\right) \\ &> g_{E_\infty}(\beta, \tau_\infty(\beta), 0) = 0, \end{aligned}$$

which is again a contradiction. Thus $\liminf_{p\to\infty} y(\beta, p) \geq y_\infty(\beta)$. We obtained that

$$\limsup_{p\to\infty} y(\beta, p) \leq y_\infty(\beta) \leq \liminf_{p\to\infty} y(\beta, p),$$

which implies that $\lim_{p\to\infty} y(\beta, p) = y_\infty(\beta)$. Thus (4.1) holds.

The property (4.2) can be proved by exactly the same argument as the proof of Lemma 2.5. The property (4.3) can be shown in the same way as [13, Lemma 2.2 (ii)]. However, we provide the proof of (4.3) for completeness. Suppose that $\liminf_{\beta\nearrow\beta_{c,\infty}} \tau_\infty(\beta) < 2\pi$. Then there exists $\varepsilon_0 \in \mathbb{R}_{>0}$ such that for any $\tilde{\beta} \in (0, \beta_{c,\infty})$

$\inf_{\beta\in[\tilde{\beta},\beta_{c,\infty})}\tau_\infty(\beta)\le 2\pi-\varepsilon_0$. Take any $\tilde{\beta}\in(0,\beta_{c,\infty})$. There exists $\beta'\in[\tilde{\beta},\beta_{c,\infty})$ such that $\tau_\infty(\beta')\le 2\pi-\frac{\varepsilon_0}{2}$, which implies that

$$0=g_{E_\infty}(\beta',\tau_\infty(\beta'),0)\le g_{E_\infty}\left(\beta',2\pi-\frac{\varepsilon_0}{2},0\right)\le\sup_{\beta\in[\tilde{\beta},\beta_{c,\infty})}g_{E_\infty}\left(\beta,2\pi-\frac{\varepsilon_0}{2},0\right).$$

Since $\tilde{\beta}$ is arbitrary,

$$0\le\limsup_{\beta\nearrow\beta_{c,\infty}}g_{E_\infty}\left(\beta,2\pi-\frac{\varepsilon_0}{2},0\right)=g_{E_\infty}\left(\beta_{c,\infty},2\pi-\frac{\varepsilon_0}{2},0\right)<g_{E_\infty}(\beta_{c,\infty},2\pi,0)=0,$$

which is a contradiction. Therefore $\liminf_{\beta\nearrow\beta_{c,\infty}}\tau_\infty(\beta)\ge 2\pi$. Since $\limsup_{\beta\nearrow\beta_{c,\infty}}\tau_\infty(\beta)\le 2\pi$, (4.3) holds. □

In the following let x_0 be that defined in (3.2), $\beta_{c,\infty}$ be that introduced in Lemma 4.2 (i) and $y_\infty(\beta):=\cos(\frac{\tau_\infty(\beta)}{2})$ ($\beta\in(0,\beta_{c,\infty})$) with $\tau_\infty(\cdot)$ introduced in Lemma 4.2 (ii). We need to prepare an analogue of Lemma 3.2 with E_∞.

Lemma 4.4. *There exists $U_0\in(0,\frac{2e_{min}}{b})$ such that the following statement holds. For any $U\in[-U_0,0)$ there exists $Y\in(-1,0)$ such that $\sqrt{1+Y}x_0\in(0,\beta_{c,\infty})$ and $y_\infty(\sqrt{1+Y}x_0)=Y$.*

Proof. By using (4.2), (4.3) in place of Lemma 2.5, Lemma 1.2 (ii) respectively we can repeat an argument parallel to the proof of Lemma 3.2 to prove the statement. □

Proving the next lemma is the most complicated in this paper.

Lemma 4.5. *Assume that $\frac{e_{min}}{e_{max}}=\sqrt{9-4\sqrt{5}}$. Then there exists $y_0\in(-1,0)$ such that $W_{E_\infty}(x_0,y)<0$ for any $y\in(-1,y_0]$.*

Let us postpone the proof of the above lemma and show Proposition 1.8 here.

Proof of Proposition 1.8. Let $y_0\in(-1,0)$ be that introduced in Lemma 4.5. For any $U\in[-\frac{e_{min}}{\sinh(2)b},0)$, $\beta\in(0,\beta_{c,\infty})$ the same inequality as the 2nd inequality of Lemma 2.4 holds with $y_\infty(\beta)$ in place of $y(\beta)$. It follows that there exists $U_0\in(0,\frac{2e_{min}}{b})$ such that $y_\infty(\beta)\in(-1,y_0]$ for any $U\in[-U_0,0)$, $\beta\in(0,\beta_{c,\infty})$. By choosing U_0 smaller if necessary we can apply Lemma 4.4 to ensure that for any $U\in[-U_0,0)$ there exists $Y\in(-1,0)$ such that $\sqrt{1+Y}x_0\in(0,\beta_{c,\infty})$ and $y_\infty(\sqrt{1+Y}x_0)=Y\in(-1,y_0]$. Let us fix $U\in[-U_0,0)$. Set $\beta':=\sqrt{1+Y}x_0$. Recalling the conclusion of Lemma 4.5,

$$0>W_{E_\infty}(x_0,Y)=W_{E_\infty}\left(\frac{\beta'}{\sqrt{1+Y}},Y\right)=W_{E_\infty}\left(\frac{\beta'}{\sqrt{1+y_\infty(\beta')}},y_\infty(\beta')\right).\tag{4.4}$$

By Lemma 4.2 (i) $\beta'\in(0,\beta_c(p))$ for any sufficiently large $p\in\mathbb{R}_{>0}$. Moreover by Lemma 4.2 (ii)

$$\lim_{p\to\infty}y(\beta',p)=y_\infty(\beta'),\tag{4.5}$$

where $y(\beta,p) := \cos(\frac{\tau(\beta,p)}{2})$ for $\beta \in (0,\beta_c(p))$. We can deduce from Lemma 4.1 and (4.5) that

$$\lim_{p\to\infty} W_{E_p}\left(\frac{\beta'}{\sqrt{1+y(\beta',p)}}, y(\beta',p)\right) = W_{E_\infty}\left(\frac{\beta'}{\sqrt{1+y_\infty(\beta')}}, y_\infty(\beta')\right).$$

This coupled with (4.4) implies that there exists $p \in \mathbb{R}_{>0}$ such that $\beta' \in (0,\beta_c(p))$ and

$$0 > W_{E_p}\left(\frac{\beta'}{\sqrt{1+y(\beta',p)}}, y(\beta',p)\right).$$

Finally the above inequality and (2.23) ensure that $\frac{d^2\tau}{d\beta^2}(\beta') < 0$ for $E = E_p$. This concludes the proof. □

4.2 Negativity of the core function

It remains to prove Lemma 4.5. More strongly we will prove the next lemma, which implies Lemma 4.5.

Lemma 4.6. *Assume that* $\frac{e_{min}}{e_{max}} = \sqrt{9-4\sqrt{5}}$. *The function* $W_{E_\infty}(x_0,\cdot) : (-1,0) \to \mathbb{R}$ *can be continued into a neighborhood of* $y=-1$ *in* $\mathbb{R}$ *as a real analytic function. If we let* $W_{E_\infty}(x_0,\cdot)$ *denote the continued function as well,*

$$W_{E_\infty}(x_0,-1) = 0,\ \frac{\partial W_{E_\infty}}{\partial y}(x_0,-1) = 0,\ \frac{1}{2}\cdot\frac{\partial^2 W_{E_\infty}}{\partial y^2}(x_0,-1) = -\frac{\sqrt{2}\cdot 5^3}{2^2\cdot 3^2}.$$

Remark 4.7. At present deducing from Lemma 4.6 is the only way to prove Lemma 4.5. We show Lemma 4.6 by long calculations, though we organize the process as much as possible. Since these derivatives eventually take simple values, there may be a nice mathematical structure leading to a substantially simpler proof. However, we are unable to reveal it. In the following we should keep in mind that any single miscalculation ruins the proof of Lemma 4.6. We add that based on (3.6), (4.6), it is straightforward to write a code to compute the low order terms of $W_{E_\infty}(x_0,\cdot)$ numerically in PC.

Recall that the partial derivatives of the function $F^\infty : \mathbb{R}_{>0}\times(-1,0) \to \mathbb{R}$ can be characterized as in (2.4), (2.5), (2.6), (2.7), (2.8). Moreover, W_{E_∞} can be written with the partial derivatives of F^∞ as in (2.22). To shorten subsequent formulas, we define the functions G_x, G_y, G_{xx}, G_{xy}, $G_{yy} : (-1,0) \to \mathbb{R}$ by

$$G_x(y) := (y+1)F^\infty_x(\sqrt{y+1}x_0, y),\ G_y(y) := \frac{(y+1)^{\frac{3}{2}}}{x_0}F^\infty_y(\sqrt{y+1}x_0, y),$$
$$G_{xx}(y) := \frac{x_0}{2}(y+1)^{\frac{3}{2}}F^\infty_{xx}(\sqrt{y+1}x_0, y),\ G_{xy}(y) := (y+1)^2F^\infty_{xy}(\sqrt{y+1}x_0, y),$$
$$G_{yy}(y) := \frac{(y+1)^{\frac{5}{2}}}{x_0}F^\infty_{yy}(\sqrt{y+1}x_0, y).$$

We can see from (2.22) that

(4.6)
$$W_{E_\infty}(x_0,y) = \frac{2}{(1-y)^{\frac{3}{2}}G_y(y)^3}$$

$$\cdot \big(-yG_x(y)^2G_y(y) + (1-y)(2G_{xx}(y)G_y(y)^2 - 2G_x(y)G_y(y)G_{xy}(y) + G_{yy}(y)G_x(y)^2)\big).$$

Moreover we set for $m, n \in \mathbb{N} \cup \{0\}$

$$C_{m,n} := D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr} \left(\frac{(\frac{x_0^2}{2}E_\infty(\mathbf{k})^2)^m}{(1+\frac{x_0^2}{2}E_\infty(\mathbf{k})^2)^n} \right).$$

By (3.6)

$$C_{m,n} = b \left(s_1 \frac{(\frac{x_0^2}{2}e_{min}^2)^m}{(1+\frac{x_0^2}{2}e_{min}^2)^n} + s_2 \frac{(\frac{x_0^2}{2}e_{max}^2)^m}{(1+\frac{x_0^2}{2}e_{max}^2)^n} \right).$$

We are going to compute $W_\infty(x_0, y)$ up to the 2nd order term of $y+1$. Let us proceed step by step.

Lemma 4.8. *The functions G_x, G_y, G_{xx}, G_{xy}, G_{yy} can be expanded into convergent power series of $y+1$ in a neighborhood of $y=-1$. Moreover, as $y \searrow -1$*

$$G_x(y) = -C_{0,1} + 2C_{0,2} + \left(\frac{C_{2,2}}{2\cdot 3} - \frac{2}{3}C_{2,3} + C_{0,1} - C_{0,2} \right)(y+1) + O((y+1)^2),$$

$$\begin{aligned} G_y(y) = &-C_{0,2} + \left(-\frac{C_{1,2}}{3} + \frac{C_{2,3}}{3} \right)(y+1) \\ &+ \left(-\frac{C_{2,2}}{2\cdot 3\cdot 5} + \frac{2}{3\cdot 5}C_{3,3} - \frac{C_{4,4}}{2^2\cdot 3} \right)(y+1)^2 + O((y+1)^3), \end{aligned}$$

$$\begin{aligned} G_{xx}(y) = &C_{1,2} - 2^2C_{1,3} \\ &+ \left(\frac{C_{2,2}}{3} - \frac{C_{3,3}}{3} - \frac{2^2}{3}C_{2,3} + 2C_{3,4} - C_{1,2} + 2C_{1,3} \right)(y+1) \end{aligned}$$

$$+ \left(\frac{C_{3,2}}{2\cdot 3\cdot 5} - \frac{2}{3\cdot 5}C_{4,3} + \frac{C_{5,4}}{2^2\cdot 3} + \frac{C_{3,3}}{5} + \frac{2^2}{5}C_{4,4} - \frac{2}{3}C_{5,5} - \frac{C_{2,2}}{3} + \frac{2}{3}C_{2,3} - C_{3,4} \right)(y+1)^2$$

$$+ O((y+1)^3),$$

$$G_{xy}(y) = 3C_{0,2} - 2^2C_{0,3} + (-C_{2,3} + 2C_{2,4} + C_{0,1} - 3C_{0,2} + 2C_{0,3})(y+1)$$

$$+ \left(-\frac{C_{3,3}}{3\cdot 5} + \frac{C_{4,4}}{2^2} + \frac{2}{3\cdot 5}C_{3,4} - \frac{2}{3}C_{4,5} - \frac{C_{2,2}}{2\cdot 3} + C_{2,3} - C_{2,4} \right)(y+1)^2 + O((y+1)^3),$$

$$\begin{aligned} G_{yy}(y) = &2C_{0,3} + \left(\frac{2}{3}C_{1,3} - C_{2,4} \right)(y+1) + \left(\frac{C_{2,3}}{3\cdot 5} - \frac{2}{5}C_{3,4} + \frac{C_{4,5}}{3} \right)(y+1)^2 \\ &+ O((y+1)^3). \end{aligned}$$

Remark 4.9. We will find that the 2nd order term of $G_x(y)$ is unnecessary to prove Lemma 4.6. So we do not characterize it here for conciseness.

Proof of Lemma 4.8. For $j \in \mathbb{N} \cup \{0\}$ let us set

$$R_j := D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr} \left(1 + \frac{\cosh(\sqrt{y+1}x_0E_\infty(\mathbf{k})) - 1}{y+1} \right)^{-j},$$

$$S_j := D_d \int_{\Gamma_\infty^*} d\mathbf{k}\, \mathrm{Tr} \left(\frac{\sinh(\sqrt{y+1}x_0E_\infty(\mathbf{k}))}{\sqrt{y+1}x_0E_\infty(\mathbf{k})} \left(1 + \frac{\cosh(\sqrt{y+1}x_0E_\infty(\mathbf{k})) - 1}{y+1} \right)^{-j} \right),$$

$$\tilde{S}_j := D_d \int_{\Gamma_\infty^*} d\mathbf{k}\,\mathrm{Tr}$$
$$\cdot\left(\frac{x_0^2}{2}E_\infty(\mathbf{k})^2\frac{\sinh(\sqrt{y+1}x_0E_\infty(\mathbf{k}))}{\sqrt{y+1}x_0E_\infty(\mathbf{k})}\left(1+\frac{\cosh(\sqrt{y+1}x_0E_\infty(\mathbf{k}))-1}{y+1}\right)^{-j}\right).$$

We can derive from (2.4), (2.5), (2.6), (2.7), (2.8) with $E = E_\infty$ that

$$G_x(y) = -R_1 + 2R_2 + (R_1 - R_2)(y+1), \tag{4.7}$$
$$G_y(y) = -S_2, \tag{4.8}$$
$$G_{xx}(y) = \tilde{S}_2 - 4\tilde{S}_3 + (-\tilde{S}_2 + 2\tilde{S}_3)(y+1), \tag{4.9}$$
$$G_{xy}(y) = 3R_2 - 4R_3 + (R_1 - 3R_2 + 2R_3)(y+1), \tag{4.10}$$
$$G_{yy}(y) = 2S_3. \tag{4.11}$$

We can see that R_j, S_j, $\tilde{S}_j$ $(j \in \mathbb{N}\cup\{0\})$ can be expanded into convergent power series of $y+1$ in a neighborhood of $y=-1$ and so can G_x, G_y, G_{xx}, G_{xy}, G_{yy}.

We want to characterize low order terms of R_j, S_j, $\tilde{S}_j$. Let us prepare formulas for this purpose. Let $x \in \mathbb{R}_{>0}$, $a \in \mathbb{R}\backslash\{0\}$, $n \in \mathbb{N}$. Set $X := \frac{x^2}{2}$, $A := a^2$. Observe that

$$\begin{aligned}
&\left(1+\frac{\cosh(\sqrt{y+1}xa)-1}{y+1}\right)^{-n}\\
&= \left(1 + XA + \frac{X^2A^2}{2\cdot 3}(y+1) + \frac{X^3A^3}{2\cdot 3^2\cdot 5}(y+1)^2\right)^{-n} + O((y+1)^3)\\
&= (1+XA)^{-n}\Bigg(1 - \frac{X^2A^2}{2\cdot 3(1+XA)}(y+1)\\
&\qquad + \left(-\frac{X^3A^3}{2\cdot 3^2\cdot 5(1+XA)} + \frac{X^4A^4}{2^2\cdot 3^2(1+XA)^2}\right)(y+1)^2\Bigg)^n + O((y+1)^3),\\
&\frac{\sinh(\sqrt{y+1}xa)}{\sqrt{y+1}xa} = 1 + \frac{XA}{3}(y+1) + \frac{X^2A^2}{2\cdot 3\cdot 5}(y+1)^2 + O((y+1)^3).
\end{aligned}$$

By using the above equalities we obtain that

$$\begin{aligned}
&\left(1+\frac{\cosh(\sqrt{y+1}xa)-1}{y+1}\right)^{-1}\\
&= \frac{1}{1+XA} - \frac{X^2A^2}{2\cdot 3(1+XA)^2}(y+1)\\
&\quad + \left(-\frac{X^3A^3}{2\cdot 3^2\cdot 5(1+XA)^2} + \frac{X^4A^4}{2^2\cdot 3^2(1+XA)^3}\right)(y+1)^2 + O((y+1)^3),\\
&\left(1+\frac{\cosh(\sqrt{y+1}xa)-1}{y+1}\right)^{-2}\\
&= \frac{1}{(1+XA)^2} - \frac{X^2A^2}{3(1+XA)^3}(y+1)\\
&\quad + \left(-\frac{X^3A^3}{3^2\cdot 5(1+XA)^3} + \frac{X^4A^4}{2^2\cdot 3(1+XA)^4}\right)(y+1)^2 + O((y+1)^3),
\end{aligned}$$

$$\left(1+\frac{\cosh(\sqrt{y+1}xa)-1}{y+1}\right)^{-3}$$
$$=\frac{1}{(1+XA)^3}-\frac{X^2A^2}{2(1+XA)^4}(y+1)$$
$$+\left(-\frac{X^3A^3}{2\cdot 3\cdot 5(1+XA)^4}+\frac{X^4A^4}{2\cdot 3(1+XA)^5}\right)(y+1)^2+O((y+1)^3),$$

(4.12)

$$\frac{\sinh(\sqrt{y+1}xa)}{\sqrt{y+1}xa}\left(1+\frac{\cosh(\sqrt{y+1}xa)-1}{y+1}\right)^{-2}$$
$$=\frac{1}{(1+XA)^2}+\left(\frac{XA}{3(1+XA)^2}-\frac{X^2A^2}{3(1+XA)^3}\right)(y+1)$$
$$+\left(\frac{X^2A^2}{2\cdot 3\cdot 5(1+XA)^2}-\frac{2X^3A^3}{3\cdot 5(1+XA)^3}+\frac{X^4A^4}{2^2\cdot 3(1+XA)^4}\right)(y+1)^2$$
$$+O((y+1)^3),$$

(4.13)

$$\frac{\sinh(\sqrt{y+1}xa)}{\sqrt{y+1}xa}\left(1+\frac{\cosh(\sqrt{y+1}xa)-1}{y+1}\right)^{-3}$$
$$=\frac{1}{(1+XA)^3}+\left(\frac{XA}{3(1+XA)^3}-\frac{X^2A^2}{2(1+XA)^4}\right)(y+1)$$
$$+\left(\frac{X^2A^2}{2\cdot 3\cdot 5(1+XA)^3}-\frac{X^3A^3}{5(1+XA)^4}+\frac{X^4A^4}{2\cdot 3(1+XA)^5}\right)(y+1)^2+O((y+1)^3).$$

It follows that

$$R_1=C_{0,1}-\frac{C_{2,2}}{2\cdot 3}(y+1)+\left(-\frac{C_{3,2}}{2\cdot 3^2\cdot 5}+\frac{C_{4,3}}{2^2\cdot 3^2}\right)(y+1)^2+O((y+1)^3),$$
$$R_2=C_{0,2}-\frac{C_{2,3}}{3}(y+1)+\left(-\frac{C_{3,3}}{3^2\cdot 5}+\frac{C_{4,4}}{2^2\cdot 3}\right)(y+1)^2+O((y+1)^3),$$
$$R_3=C_{0,3}-\frac{C_{2,4}}{2}(y+1)+\left(-\frac{C_{3,4}}{2\cdot 3\cdot 5}+\frac{C_{4,5}}{2\cdot 3}\right)(y+1)^2+O((y+1)^3),$$
$$S_2=C_{0,2}+\left(\frac{C_{1,2}}{3}-\frac{C_{2,3}}{3}\right)(y+1)+\left(\frac{C_{2,2}}{2\cdot 3\cdot 5}-\frac{2}{3\cdot 5}C_{3,3}+\frac{C_{4,4}}{2^2\cdot 3}\right)(y+1)^2$$
$$+O((y+1)^3),$$
$$S_3=C_{0,3}+\left(\frac{C_{1,3}}{3}-\frac{C_{2,4}}{2}\right)(y+1)+\left(\frac{C_{2,3}}{2\cdot 3\cdot 5}-\frac{C_{3,4}}{5}+\frac{C_{4,5}}{2\cdot 3}\right)(y+1)^2$$
$$+O((y+1)^3),$$
$$\tilde{S}_2=C_{1,2}+\left(\frac{C_{2,2}}{3}-\frac{C_{3,3}}{3}\right)(y+1)+\left(\frac{C_{3,2}}{2\cdot 3\cdot 5}-\frac{2}{3\cdot 5}C_{4,3}+\frac{C_{5,4}}{2^2\cdot 3}\right)(y+1)^2$$
$$+O((y+1)^3),$$
$$\tilde{S}_3=C_{1,3}+\left(\frac{C_{2,3}}{3}-\frac{C_{3,4}}{2}\right)(y+1)+\left(\frac{C_{3,3}}{2\cdot 3\cdot 5}-\frac{C_{4,4}}{5}+\frac{C_{5,5}}{2\cdot 3}\right)(y+1)^2$$
$$+O((y+1)^3).$$

We can characterize $\tilde{S}_2$, $\tilde{S}_3$ as above by multiplying both sides of (4.12), (4.13) by

XA. By substituting the above equalities into (4.7), (4.8), (4.9), (4.10), (4.11) we can derive the claimed equalities. □

Next we compute each low order term of G_x, G_y, G_{xx}, G_{xy}, G_{yy}. To this end, let us compute $C_{m,n}$ for all the necessary indices m, n as efficiently as possible. The following relations help us do so.

Lemma 4.10. *(i) For any $m, n \in \mathbb{N}_{\geq 1}$ $C_{m,n} = C_{m-1,n-1} - C_{m-1,n}$.*

(ii) For any $m, n \in \mathbb{N}$ with $m \geq 2$, $n \geq 3$

$$C_{m,n} = \frac{5}{2^6} C_{m-2,n-3}.$$

Proof. (i): Use the equality $x^m = x^{m-1}(x+1) - x^{m-1}$ in the numerator of the integrand.

(ii): Since $(\frac{3-\sqrt{5}}{2})^3 = 9 - 4\sqrt{5}$,

$$\left(\frac{e_{min}}{e_{max}}\right)^{\frac{2}{3}} = \frac{3-\sqrt{5}}{2}, \quad \left(\frac{e_{max}}{e_{min}}\right)^{\frac{2}{3}} = \frac{3+\sqrt{5}}{2}. \tag{4.14}$$

Recalling the definition (3.2) and substituting (4.14), we can derive that

$$\left(1 + \frac{x_0^2}{2} e_{min}^2\right)^{-1} = \left(1 + \left(\frac{e_{min}}{e_{max}}\right)^{\frac{2}{3}} + \left(\frac{e_{min}}{e_{max}}\right)^{\frac{4}{3}}\right)^{-1} = \frac{3+\sqrt{5}}{8}, \tag{4.15}$$
$$\left(1 + \frac{x_0^2}{2} e_{max}^2\right)^{-1} = \left(1 + \left(\frac{e_{max}}{e_{min}}\right)^{\frac{2}{3}} + \left(\frac{e_{max}}{e_{min}}\right)^{\frac{4}{3}}\right)^{-1} = \frac{3-\sqrt{5}}{8}.$$

Moreover, these imply that

$$\left(1 + \frac{x_0^2}{2} e_{min}^2\right)^{-2} = \frac{7+3\sqrt{5}}{32}, \quad \left(1 + \frac{x_0^2}{2} e_{max}^2\right)^{-2} = \frac{7-3\sqrt{5}}{32}, \tag{4.16}$$
$$\left(1 + \frac{x_0^2}{2} e_{min}^2\right)^{-3} = \frac{9+4\sqrt{5}}{64}, \quad \left(1 + \frac{x_0^2}{2} e_{max}^2\right)^{-3} = \frac{9-4\sqrt{5}}{64}.$$

Therefore

$$\frac{(\frac{x_0^2}{2} e_{min}^2)^2}{(1 + \frac{x_0^2}{2} e_{min}^2)^3} = \left(1 + \frac{x_0^2}{2} e_{min}^2\right)^{-1} - 2\left(1 + \frac{x_0^2}{2} e_{min}^2\right)^{-2} + \left(1 + \frac{x_0^2}{2} e_{min}^2\right)^{-3} = \frac{5}{2^6},$$

Similarly

$$\frac{(\frac{x_0^2}{2} e_{max}^2)^2}{(1 + \frac{x_0^2}{2} e_{max}^2)^3} = \frac{5}{2^6}.$$

These equalities ensure the claimed result. □

We can achieve our purpose by using the values of $C_{m,n}$ given in the next lemma.

Lemma 4.11. *Some of $C_{m,n}/b$ $(m, n \in \mathbb{N} \cup \{0\})$ are computed as follows.*

	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
$m=0$	1	$\frac{1}{2^3}$	$\frac{1}{2^5}$	$\frac{1}{2^6}$		
$m=1$	3^2	$\frac{7}{2^3}$	$\frac{3}{2^5}$	$\frac{1}{2^6}$		
$m=2$		$\frac{5\cdot 13}{2^3}$	$\frac{5^2}{2^5}$	$\frac{5}{2^6}$	$\frac{5}{2^9}$	
$m=3$			$\frac{5\cdot 47}{2^5}$	$\frac{3^2\cdot 5}{2^6}$	$\frac{5\cdot 7}{2^9}$	
$m=4$				$\frac{5^2\cdot 17}{2^6}$	$\frac{5^2\cdot 13}{2^9}$	$\frac{5^3}{2^{11}}$
$m=5$					$\frac{3\cdot 5^2\cdot 41}{2^9}$	$\frac{5^2\cdot 47}{2^{11}}$

Remark 4.12. Though it is technically possible to compute $C_{m,n}$ for all $m, n \in \{0, 1, \cdots, 5\}$, we present only those necessary for our purpose.

Proof of Lemma 4.11. We can see that once $C_{0,n}$ $(n = 0, 1, 2, 3)$, $C_{1,0}$ are obtained, the rest can be derived by recursively applying the formulas proved in Lemma 4.10. Let us explain how to compute $C_{0,n}$ $(n = 0, 1, 2, 3)$, $C_{1,0}$. Recalling (2.33), we set $A_1 := e_{min}^2$, $A_2 := e_{max}^2$, $X := \alpha(A_1, A_2)$. It follows that $\frac{x_0^2}{2} = \alpha(A_1, A_2)$. First we need to compute s_1, s_2 defined in (3.5). The terms B_1^m, B_2^m $(m = 1, 2, 3)$ have already been obtained in (4.15), (4.16). By using them we have that

$$
\begin{aligned}
D_{1,1} &= B_1^3 = \frac{9 + 4\sqrt{5}}{64}, \\
D_{1,2} &= \frac{1}{2} B_1 B_2 (8 B_1 B_2 + B_1 + B_2 - 4B_1^2 - 4B_2^2) = -\frac{1}{64},
\end{aligned}
$$

which yield that

$$
s_1 = \frac{5 - 2\sqrt{5}}{10}, \quad s_2 = \frac{5 + 2\sqrt{5}}{10}.
$$

We can combine these with the equalities $\frac{1}{b} C_{0,n} = s_1 B_1^n + s_2 B_2^n$ $(n = 0, 1, 2, 3)$ to obtain the claimed values. Moreover, by (4.15)

$$
\frac{x_0^2}{2} e_{min}^2 = 5 - 2\sqrt{5}, \quad \frac{x_0^2}{2} e_{max}^2 = 5 + 2\sqrt{5},
$$

and thus

$$
\frac{1}{b} C_{1,0} = s_1 \frac{x_0^2}{2} e_{min}^2 + s_2 \frac{x_0^2}{2} e_{max}^2 = 3^2.
$$

□

By substituting the values presented in Lemma 4.11 into the formulas listed in Lemma 4.8 we have the following.

Lemma 4.13. *As* $y \searrow -1$,

$$\begin{aligned}
\frac{1}{b}G_x(y) &= -\frac{1}{2^4} + \frac{11}{2^6}(y+1) + O((y+1)^2),\\
\frac{1}{b}G_y(y) &= -\frac{1}{2^5} - \frac{1}{2^6\cdot 3}(y+1) + \frac{7\cdot 13}{2^{11}\cdot 3}(y+1)^2 + O((y+1)^3),\\
\frac{1}{b}G_{xx}(y) &= \frac{1}{2^5} - \frac{1}{2^8}(y+1) - \frac{3\cdot 103}{2^{11}}(y+1)^2 + O((y+1)^3),\\
\frac{1}{b}G_{xy}(y) &= \frac{1}{2^5} + \frac{1}{2^8}(y+1) + \frac{113}{2^{11}\cdot 3}(y+1)^2 + O((y+1)^3),\\
\frac{1}{b}G_{yy}(y) &= \frac{1}{2^5} + \frac{1}{2^9\cdot 3}(y+1) - \frac{11}{2^{11}\cdot 3}(y+1)^2 + O((y+1)^3).
\end{aligned}$$

Finally we can prove Lemma 4.6.

Proof of Lemma 4.6. The claim concerning the analytic continuation into a neighborhood of $y=-1$ is implied by the equality (4.6), the initial statement of Lemma 4.8 and the fact $G_y(-1)\neq 0$. Let us compute 0th, 1st and 2nd order term in the expansion of $W_{E_\infty}(x_0,y)$ with respect to $y+1$. Set for $y\in\mathbb{R}_{<0}$ close to -1

$$\begin{aligned}
J(y) :=& - yG_x(y)^2G_y(y)\\
&+ (1-y)\big(2G_{xx}(y)G_y(y)^2 - 2G_x(y)G_y(y)G_{xy}(y) + G_{yy}(y)G_x(y)^2\big),
\end{aligned}$$

so that

$$W_{E_\infty}(x_0,y) = \frac{2}{(1-y)^{\frac{3}{2}}G_y(y)^3}J(y). \tag{4.17}$$

We will see that it suffices to compute $J(-1)$, $\frac{dJ}{dy}(-1)$, $\frac{1}{2!}\frac{d^2J}{dy^2}(-1)$ to achieve our goal. Set

$$\tilde{G}(y) := 2G_{xx}(y)G_y(y)^2 - 2G_x(y)G_y(y)G_{xy}(y) + G_{yy}(y)G_x(y)^2$$

for simplicity. Observe that

$$J(y) = G_x(y)^2G_y(y) + 2\tilde{G}(y) + (y+1)\big(-G_x(y)^2G_y(y) - \tilde{G}(y)\big). \tag{4.18}$$

In the following for any smooth function f of y and $j\in\mathbb{N}\cup\{0\}$ $f^{(j)}$ denotes $\frac{1}{j!}\frac{d^jf}{dy^j}(-1)$. By Lemma 4.13

$$\frac{1}{b^3}\tilde{G}^{(0)} = \frac{1}{2^{14}}, \quad \frac{1}{b^3}(G_x^2G_y)^{(0)} = \frac{1}{b^3}(G_x^{(0)})^2G_y^{(0)} = -\frac{1}{2^{13}}. \tag{4.19}$$

Thus

$$\frac{1}{b^3}J^{(0)} = \frac{1}{b^3}\big((G_x^2G_y)^{(0)} + 2\tilde{G}^{(0)}\big) = 0.$$

Moreover, by using the 0th order terms and then the 1st order terms given in Lemma 4.13

(4.20)

$$\frac{1}{b^3}\tilde{G}^{(1)} = \frac{1}{b^3}\big(2G_{xx}^{(1)}(G_y^{(0)})^2 + 2^2G_{xx}^{(0)}G_y^{(0)}G_y^{(1)} - 2G_x^{(1)}G_y^{(0)}G_{xy}^{(0)} - 2G_x^{(0)}G_y^{(1)}G_{xy}^{(0)}$$

$$- 2G_x^{(0)}G_y^{(0)}G_{xy}^{(1)} + G_{yy}^{(1)}(G_x^{(0)})^2 + 2G_{yy}^{(0)}G_x^{(0)}G_x^{(1)})$$
$$= \frac{1}{b}\left(\frac{1}{2^9}G_{xx}^{(1)} - \frac{1}{2^9}G_x^{(1)} - \frac{1}{2^8}G_{xy}^{(1)} + \frac{1}{2^8}G_{yy}^{(1)}\right) = -\frac{5\cdot 7}{2^{15}\cdot 3},$$

(4.21)

$$\frac{1}{b^3}(G_x^2G_y)^{(1)} = \frac{1}{b^3}\big(2G_x^{(1)}G_x^{(0)}G_y^{(0)} + (G_x^{(0)})^2G_y^{(1)}\big) = \frac{1}{b}\left(\frac{1}{2^8}G_x^{(1)} + \frac{1}{2^8}G_y^{(1)}\right) = \frac{1}{2^9\cdot 3}.$$

Substitution of (4.19), (4.20), (4.21) yields that

$$\frac{1}{b^3}J^{(1)} = \frac{1}{b^3}\big((G_x^2G_y)^{(1)} + 2\tilde{G}^{(1)} - (G_x^2G_y)^{(0)} - \tilde{G}^{(0)}\big) = 0.$$

Let us compute $J^{(2)}$. By (4.18)

(4.22)

$$J^{(2)}$$
$$= (G_x^2G_y)^{(2)} + 2\big(2(G_{xx}G_y^2)^{(2)} - 2(G_xG_yG_{xy})^{(2)} + (G_{yy}G_x^2)^{(2)}\big) - (G_x^2G_y)^{(1)} - \tilde{G}^{(1)}.$$

Let us decompose each term with the superscript "(2)" in the right-hand side of (4.22) by using the 0th order terms given in Lemma 4.13.

(4.23)

$$\frac{1}{b^3}(G_x^2G_y)^{(2)} = \frac{1}{b^3}\big(2G_x^{(2)}G_x^{(0)}G_y^{(0)} + (G_x^{(0)})^2G_y^{(2)} + (G_x^{(1)})^2G_y^{(0)} + 2G_x^{(1)}G_x^{(0)}G_y^{(1)}\big)$$
$$= \frac{1}{b}\left(\frac{1}{2^8}G_x^{(2)} + \frac{1}{2^8}G_y^{(2)}\right) + \frac{1}{b^2}\left(-\frac{1}{2^5}(G_x^{(1)})^2 - \frac{1}{2^3}G_x^{(1)}G_y^{(1)}\right),$$

(4.24)

$$\frac{1}{b^3}(G_{xx}G_y^2)^{(2)} = \frac{1}{b^3}\big(G_{xx}^{(2)}(G_y^{(0)})^2 + 2G_{xx}^{(0)}G_y^{(2)}G_y^{(0)} + 2G_{xx}^{(1)}G_y^{(1)}G_y^{(0)} + G_{xx}^{(0)}(G_y^{(1)})^2\big)$$
$$= \frac{1}{b}\left(\frac{1}{2^{10}}G_{xx}^{(2)} - \frac{1}{2^9}G_y^{(2)}\right) + \frac{1}{b^2}\left(-\frac{1}{2^4}G_{xx}^{(1)}G_y^{(1)} + \frac{1}{2^5}(G_y^{(1)})^2\right),$$

(4.25)

$$\frac{1}{b^3}(G_xG_yG_{xy})^{(2)} = \frac{1}{b^3}\big(G_x^{(2)}G_y^{(0)}G_{xy}^{(0)} + G_x^{(0)}G_y^{(2)}G_{xy}^{(0)} + G_x^{(0)}G_y^{(0)}G_{xy}^{(2)} + G_x^{(1)}G_y^{(1)}G_{xy}^{(0)}$$
$$+ G_x^{(1)}G_y^{(0)}G_{xy}^{(1)} + G_x^{(0)}G_y^{(1)}G_{xy}^{(1)}\big)$$
$$= \frac{1}{b}\left(-\frac{1}{2^{10}}G_x^{(2)} - \frac{1}{2^9}G_y^{(2)} + \frac{1}{2^9}G_{xy}^{(2)}\right)$$
$$+ \frac{1}{b^2}\left(\frac{1}{2^5}G_x^{(1)}G_y^{(1)} - \frac{1}{2^5}G_x^{(1)}G_{xy}^{(1)} - \frac{1}{2^4}G_y^{(1)}G_{xy}^{(1)}\right),$$

(4.26)

$$\frac{1}{b^3}(G_{yy}G_x^2)^{(2)} = \frac{1}{b^3}\big(G_{yy}^{(2)}(G_x^{(0)})^2 + 2G_{yy}^{(0)}G_x^{(2)}G_x^{(0)} + 2G_{yy}^{(1)}G_x^{(1)}G_x^{(0)} + G_{yy}^{(0)}(G_x^{(1)})^2\big)$$
$$= \frac{1}{b}\left(\frac{1}{2^8}G_{yy}^{(2)} - \frac{1}{2^8}G_x^{(2)}\right) + \frac{1}{b^2}\left(-\frac{1}{2^3}G_{yy}^{(1)}G_x^{(1)} + \frac{1}{2^5}(G_x^{(1)})^2\right).$$

By substituting (4.20), the 2nd equality of (4.21), (4.23), (4.24), (4.25), (4.26) into (4.22)

(4.27)

$$\frac{1}{b^3}J^{(2)} = \frac{1}{b}\left(\frac{1}{2^8}G_y^{(2)} + \frac{1}{2^8}G_{xx}^{(2)} - \frac{1}{2^7}G_{xy}^{(2)} + \frac{1}{2^7}G_{yy}^{(2)}\right)$$

$$
\begin{aligned}
&+\frac{1}{b^2}\Big(\frac{1}{2^5}(G_x^{(1)})^2-\frac{1}{2^2}G_x^{(1)}G_y^{(1)}-\frac{1}{2^2}G_{xx}^{(1)}G_y^{(1)}+\frac{1}{2^3}(G_y^{(1)})^2+\frac{1}{2^3}G_x^{(1)}G_{xy}^{(1)}\\
&\qquad+\frac{1}{2^2}G_y^{(1)}G_{xy}^{(1)}-\frac{1}{2^2}G_{yy}^{(1)}G_x^{(1)}\Big)\\
&+\frac{1}{b}\left(-\frac{1}{2^8}G_x^{(1)}-\frac{1}{2^8}G_y^{(1)}\right)+\frac{5\cdot 7}{2^{15}\cdot 3}\\
=&\ \frac{1}{b}\left(\frac{1}{2^8}G_y^{(2)}+\frac{1}{2^8}G_{xx}^{(2)}-\frac{1}{2^7}G_{xy}^{(2)}+\frac{1}{2^7}G_{yy}^{(2)}\right)\\
&+\frac{1}{b}G_x^{(1)}\left(\frac{1}{b}\left(\frac{1}{2^5}G_x^{(1)}-\frac{1}{2^2}G_y^{(1)}+\frac{1}{2^3}G_{xy}^{(1)}-\frac{1}{2^2}G_{yy}^{(1)}\right)-\frac{1}{2^8}\right)\\
&+\frac{1}{b}G_y^{(1)}\left(\frac{1}{b}\left(-\frac{1}{2^2}G_{xx}^{(1)}+\frac{1}{2^3}G_y^{(1)}+\frac{1}{2^2}G_{xy}^{(1)}\right)-\frac{1}{2^8}\right)+\frac{5\cdot 7}{2^{15}\cdot 3}.
\end{aligned}
$$

We remark that $G_x^{(2)}$ is canceled here. By applying Lemma 4.13 again we have that

$$
\begin{aligned}
\text{(1st term of R.H.S of (4.27))} &= -\frac{271}{2^{17}\cdot 3},\\
\text{(2nd term of R.H.S of (4.27))} &= \frac{11\cdot 19}{2^{17}\cdot 3},\\
\text{(3rd term of R.H.S of (4.27))} &= \frac{1}{2^{13}\cdot 3^2}.
\end{aligned}
$$

Therefore

$$
\frac{1}{b^3}J^{(2)}=-\frac{271}{2^{17}\cdot 3}+\frac{11\cdot 19}{2^{17}\cdot 3}+\frac{1}{2^{13}\cdot 3^2}+\frac{5\cdot 7}{2^{15}\cdot 3}=\frac{5^3}{2^{16}\cdot 3^2}.
$$

By combining the above results with (4.17) and the equality

$$
\frac{2}{(1-y)^{\frac{3}{2}}G_y(y)^3}=\frac{1}{\sqrt{2}(G_y^{(0)})^3}+O((y+1))
$$

we see that as $y\searrow -1$

$$
\begin{aligned}
W_{E_\infty}(x_0,y)&=\frac{1}{\sqrt{2}(G_y^{(0)})^3}J^{(2)}(y+1)^2+O((y+1)^3)\\
&=-\frac{\sqrt{2}\cdot 5^3}{2^2\cdot 3^2}(y+1)^2+O((y+1)^3).
\end{aligned}
$$

This implies the results. □

References

[1] N. O. Abeling and S. Kehrein, Quantum quench dynamics in the transverse field Ising model at nonzero temperatures, Phys. Rev. B **93** (2016), 104302.

[2] N. N. Bogolyubov, Jr, A method for studying model hamiltonians: A minimax principle for problems in statistical physics, International Series of Monographs in Natural Philosophy **43**, Pergamon Press, Oxford, 1972.

[3] U. Bhattacharya, S. Bandyopadhyay and A. Dutta, Mixed state dynamical quantum phase transitions, Phys. Rev. B **96** (2017), 180303(R).

[4] A. Dembo and O. Zeitouni, Large deviations techniques and applications, second edition, Stochastic Modelling and Applied Probability **38**, Springer-Verlag, Berlin, Heidelberg, 1998.

[5] F. D. M. Haldane, Model for a quantum Hall effect without Landau levels: Condensed-matter realization of the "parity anomaly", Phys. Rev. Lett. **61** (1988), 2015.

[6] J. C. Halimeh and V. Zauner-Stauber, Dynamical phase diagram of quantum spin chains with long-range interactions, Phys. Rev. B **96** (2017), 134427.

[7] M. Heyl, Dynamical quantum phase transitions: a review, Rep. Prog. Phys. **81** (2018), 054001.

[8] M. Heyl and J. C. Budich, Dynamical topological quantum phase transitions for mixed states, Phys. Rev. B **96** (2017), 180304(R).

[9] M. Heyl, A. Polkovnikov and S. Kehrein, Dynamical quantum phase transitions in the transverse-field Ising model, Phys. Rev. Lett. **110** (2013), 135704.

[10] X. Y. Hou, Q. C. Gao, H. Guo and C. C. Chien, Metamorphic dynamical quantum phase transition in double-quench processes at finite temperatures, Phys. Rev. B **106** (2022), 014301.

[11] Y. Kashima, Superconducting phase in the BCS model with imaginary magnetic field, J. Math. Sci. Univ. Tokyo **28** (2021), 1–179.

[12] Y. Kashima, Superconducting phase in the BCS model with imaginary magnetic field. II. Multi-scale infrared analysis, J. Math. Sci. Univ. Tokyo **28** (2021), 181–398.

[13] Y. Kashima, Superconducting phase in the BCS model with imaginary magnetic field. III. Non-vanishing free dispersion relations, J. Math. Sci. Univ. Tokyo **28** (2021), 399–556.

[14] Y. Kashima, Higher order phase transitions in the BCS model with imaginary magnetic field, J. Math. Sci. Univ. Tokyo **30** (2023), 125–203. The preprint version is available in https://natmathexplab.org

[15] S. G. Krantz and H. R. Parks, A primer of real analytic functions, 2nd edition, Birkhäuser, 2002.

[16] J. Lang, B. Frank and J. C. Halimeh, Concurrence of dynamical phase transitions at finite temperature in the fully connected transverse-field Ising model, Phys. Rev. B **97** (2018), 174401.

[17] B. Mera, C. Vlachou, N. Paunković, V. R. Vieira and O. Viyuela, Dynamical phase transitions at finite temperature from fidelity and interferometric Loschmidt echo induced metrics, Phys. Rev. B **97** (2018), 094110.

[18] H. P. Ojeda Collado, G. Usaj, C. A. Balseiro, D. H. Zanette and J. Lorenzana, Dynamical phase transitions in periodically driven Bardeen-Cooper-Schrieffer systems, Phys. Rev. Res. **5** (2023), 023014.

[19] C. Rylands, E. A. Yuzbashyan, V. Gurarie, A. Zabalo and V. Galitski, Loschmidt echo of far-from-equilibrium fermionic superfluids, Ann. Phys. **435** (2021), 168554.

[20] N. Sedlmayr, M. Fleischhauer and J. Sirker, Fate of dynamical phase transitions at finite temperatures and in open systems, Phys. Rev. B **97** (2018), 045147.

[21] A. Silva, Statistics of the work done on a quantum critical system by quenching a control parameter, Phys. Rev. Lett. **101** (2008), 120603.

[22] W. P. Su, J. R. Schrieffer and A. J. Heeger, Solitons in Polyacetylene, Phys. Rev. Lett. **42** (1979), 1698.

[23] P. Talkner, E. Lutz and P. Hänggi, Fluctuation theorems: Work is not an observable, Phys. Rev. E **75** (2007), 050102(R).

[24] D. J. Young, A. Chu, E. Y. Song, D. Barberena, D. Wellnitz, Z. Niu, V. M. Schäfer, R. J. Lewis-Swan, A. M. Rey and J. K. Thompson, Observing dynamical phases of BCS superconductors in a cavity QED simulator, Nature **625** (2024), 679–684.

[25] B. Žunkovič, M. Heyl, M. Knap and A. Silva, Dynamical quantum phase transitions in spin chains with long-range interactions: Merging different concepts of nonequilibrium criticality, Phys. Rev. Lett. **120** (2018), 130601.