

# Higher order phase transitions in the BCS model with imaginary magnetic field

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## Abstract

In the BCS model with imaginary magnetic field at positive temperature we provide necessary and sufficient conditions for existence of a higher order phase transition driven by temperature. We define the order of the phase transition by regularity of the extended free energy density with temperature. More precisely we prove the following. There exist a non-vanishing free dispersion relation and a weak coupling constant such that a temperature-driven phase transition of order  $n \in 4\mathbb{N} + 2$  ( $= \{6, 10, 14, \dots\}$ ) occurs if and only if the minimum of the magnitude of the free dispersion relation over the maximum is less than or equal to the critical value  $\sqrt{17 - 12\sqrt{2}}$ . These statements are also proved to be equivalent to that there exist a non-vanishing free dispersion relation and a weak coupling constant such that the phase boundary varying with the inverse temperature has a stationary point of inflection. Moreover, it follows that for any non-vanishing free dispersion relation and weak coupling constant the temperature-driven phase transition is of 2nd order if and only if the minimum of the magnitude of the free dispersion relation over the maximum is larger than  $\sqrt{17 - 12\sqrt{2}}$ . We apply some key lemmas established in Section 2 of [Y. Kashima, J. Math. Sci. Univ. Tokyo **28** (2021), 399–556]. So this work is a continuation of the section of the preceding paper. \*

## 1 Introduction and main results

### 1.1 Introduction

The infinite-volume limit of the many-electron system governed by the Bardeen-Cooper-Schrieffer (BCS) model with imaginary magnetic field can be explicitly

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derived for any positive temperature and weak coupling constant if the free dispersion relation is non-vanishing, as shown in the preceding work [25]. While the temperature, the imaginary magnetic field and the coupling constant are largely restricted in [23], where the free Fermi surface is non-degenerate, and in [24], where the free Fermi surface is typically degenerate but non-empty, we have more freedom to choose these parameters in the framework of [25]. In particular, if the coupling constant is sufficiently small depending on the non-vanishing free dispersion relation, we can fully draw the phase boundary in the 2D plane of (inverse temperature, imaginary magnetic field) and justify the derivation of the infinite-volume limit of the free energy density at the same time. This means that we can reach a rigorous conclusion on the phase transitions happening in the infinite-volume limit of the many-electron system by means of mathematical analysis of the phase boundary. This is what we aim for in this paper.

The imaginary magnetic field can be considered as the real time variable in the context of dynamical quantum phase transition (DQPT). This fact motivates us to establish fundamental properties of this unconventional BCS model. The physical research on DQPT has been growing steadily since the proposal [18]. Let us summarize the formalism of DQPT to which our free energy density is related. DQPT at zero temperature is defined as appearance of non-analyticity of the function

$$(1.1) \quad t \mapsto \lim_{N \rightarrow \infty} \frac{1}{N} \log \langle \psi_0, e^{-itH} \psi_0 \rangle,$$

where  $H$  is a quantum many-body Hamiltonian,  $\psi_0$  is a state vector and  $N$  denotes the system size ([18], [15]). The quantity  $\langle \psi_0, e^{-itH} \psi_0 \rangle$  is called the Loschmidt amplitude, which measures the overlap between the initial state and the state after time-evolution. There have been attempts to generalize the concept to finite temperature. When  $\psi_0$  is the ground state of a Hamiltonian  $H_0$ , the finite-temperature counterpart of the Loschmidt amplitude is

$$(1.2) \quad \frac{\text{Tr}(e^{-\beta H_0} e^{-itH})}{\text{Tr } e^{-\beta H_0}}$$

with the inverse temperature  $\beta (\in \mathbb{R}_{>0})$ . Accordingly DQPT at positive temperature is defined by non-analyticity of the function

$$(1.3) \quad t \mapsto \lim_{N \rightarrow \infty} \frac{1}{N} \log \left( \frac{\text{Tr}(e^{-\beta H_0} e^{-itH})}{\text{Tr } e^{-\beta H_0}} \right)$$

(see e.g. [3], [17], [31], [20], [19]). There is another approach to DQPT at positive temperature. It is known ([37], [35]) that the characteristic function of the work done in a quantum system where the initial Hamiltonian  $H_0$  suddenly changes to  $H_1$  is given by

$$(1.4) \quad \frac{\text{Tr}(e^{-\beta H_0} e^{-itH_0} e^{itH_1})}{\text{Tr } e^{-\beta H_0}}.$$

As pointed out in [35], (1.4) is also considered as a finite-temperature version of the Loschmidt amplitude  $\langle \psi_0, e^{-itH_0} e^{itH_1} \psi_0 \rangle$ . In [1], [34], [33] there are explanations about defining DQPT at positive temperature based on (1.4) in place of (1.2). Let us explain how our model fits in these formalism. Let  $\mathsf{H}$  denote the BCS model

and  $\mathbf{S}_z$  denote the  $z$ -component of the spin operator. The explicit definition will be given in Subsection 1.2. In this paper we analyze the free energy density of the BCS model with imaginary magnetic field

$$(1.5) \quad \lim_{N \rightarrow \infty} \left( -\frac{1}{\beta N} \log(\mathrm{Tr} e^{-\beta \mathbf{H} + it \mathbf{S}_z}) \right).$$

Within the weak coupling regime of this paper no temperature-driven phase transition is signaled as singularity of the free energy density without imaginary magnetic field

$$\lim_{N \rightarrow \infty} \left( -\frac{1}{\beta N} \log(\mathrm{Tr} e^{-\beta \mathbf{H}}) \right).$$

Thus the regularity of (1.5) with  $(\beta, t)$  in  $\mathbb{R}_{>0} \times \mathbb{R}$  is the same as that of

$$\lim_{N \rightarrow \infty} \left( -\frac{1}{\beta N} \log \left( \frac{\mathrm{Tr} e^{-\beta \mathbf{H} + it \mathbf{S}_z}}{\mathrm{Tr} e^{-\beta \mathbf{H}}} \right) \right).$$

Since  $\mathbf{S}_z$  commutes with  $\mathbf{H}$ ,

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

We can see that analyzing (1.5) is linked to the study of DQPT at positive temperature based on both (1.2) and (1.4). Jump discontinuity of the 2nd order time derivative of (1.5) was shown in [25, Proposition 2.5 (iii)], which therefore implies a DQPT in the BCS model at positive temperature. This phenomenon has not been reported in other articles except for our previous work, to the best of the author's knowledge.

One main theme of the physical research on DQPT so far is the possible relation between DQPT and equilibrium phase transition (EPT). In (1.1) with the ground state vector  $\psi_0$  of a Hamiltonian  $H_0$  or in (1.3) the question is whether existence of a DQPT is related to existence of an EPT in the systems governed by  $H_0$ ,  $H$ . One expected scenario is that a DQPT occurs if  $H_0$  and  $H$  are in mutually distinct phases so that the quench from  $H_0$  to  $H$  crosses a critical point of EPT. In the formulation (1.4) the quench is from  $H_0$  to  $H_1$ . Thus the same question with  $H_1$  in place of  $H$  should be considered. As summarized in the review article [15], there are many results indicating such correspondences between DQPT and EPT. For example the article [3] shows that a DQPT occurs based on the formulation (1.3) with the transverse-field Ising chain if the quench of the transverse magnetic field crosses a quantum critical point, which is a critical point of EPT at zero temperature. The article [17] presents a DQPT in the formulation of the type (1.3) with the 2D massive Dirac model after quenching across a critical point of topological phase transition. On the other hand, there are also many DQPTs unrelated to EPT. For example the papers [2], [40] highlight occurrence of DQPTs without crossing any EPT in quantum spin chains at zero temperature. As for positive temperature, the paper [31] intends to present numerical results showing DQPTs based on the formulation (1.3) for the fully connected transverse-field Ising model, despite that the quench from  $H_0$  to  $H$  does not cross any equilibrium critical point, in Appendix B. See the arXiv version of [31, Appendix B] for clean presentation. As emphasized in [15], DQPT seems to be a critical phenomena

which is not tightly connected with EPT in general. We know that DQPTs occur in the formulation (1.4) when  $H_0$  is the weakly interacting BCS model  $\mathsf{H}$  and  $H_1 = \mathsf{H} + \mathbf{S}_z$  at high temperatures. We can deduce from the definition of DQPT that the same conclusion holds for  $H_1 = \mathsf{H} + \theta \mathbf{S}_z$  for any  $\theta \in \mathbb{R} \setminus \{0\}$ . It is possible to reconstruct the framework [23] to prove that if the BCS interaction is weak and the temperature is high,  $\mathsf{H} + \theta \mathbf{S}_z$  is in a trivial phase without  $U(1)$ -symmetry breaking for any  $\theta \in \mathbb{R}$ . See Remark 1.14 for the technical details. In summary the DQPTs occur despite that the quench from  $\mathsf{H}$  to  $\mathsf{H} + \theta \mathbf{S}_z$  crosses no critical point of EPT. As explained above, finding no clear relation between our DQPTs and the typical EPTs in the BCS model is not discouraging. It is rather interesting that DQPTs characterized by spontaneous  $U(1)$ -symmetry breaking occur at high temperatures (see [25, Theorem 1.3]) where such an order cannot exist in the equilibrium case.

There is yet another definition of DQPT at positive temperature, based on the fidelity between the initial thermal density operator  $\rho(0)$  and the density operator  $\rho(t)$  after time evolution, where

$$\rho(t) := \frac{e^{-itH} e^{-\beta H_0} e^{itH}}{\text{Tr } e^{-\beta H_0}}, \quad t \in \mathbb{R}$$

with Hamiltonians  $H_0, H$ . The DQPT is defined as non-analyticity of the function

$$t \mapsto \lim_{N \rightarrow \infty} \frac{1}{N} \log \text{Tr} \left( \sqrt{\sqrt{\rho(0)} \rho(t) \sqrt{\rho(0)}} \right).$$

See e.g. [33], [31], [34] for the definition. The fidelity version of DQPT in our model is defined with

$$\rho(t) = \frac{e^{-it\mathbf{S}_z} e^{-\beta \mathsf{H}} e^{it\mathbf{S}_z}}{\text{Tr } e^{-\beta \mathsf{H}}}, \quad t \in \mathbb{R}.$$

However, since  $\mathsf{H}$  commutes with  $\mathbf{S}_z$ ,  $\rho(t) = \rho(0)$  for all  $t \in \mathbb{R}$ . This implies non-existence of DQPT in the fidelity-based formulation. This is not an uncommon scenario. The paper [20] features a couple of multi-band non-hopping models which show DQPTs in the formulation (1.3) with finite  $\beta$  or in the infinite-temperature limit  $\beta \rightarrow 0$ , despite that the initial density operator is unchanged by quantum quench, or in short  $\rho(t) = \rho(0)$  for any  $t \in \mathbb{R}$ , and thus there is no DQPT in the fidelity-based formulation. In general the finite-temperature Loschmidt amplitude (1.2), (1.4) can be reformulated into the overlap between time-evolving pure states via purification of the initial density operator. The paper [20] attempts to give a physical interpretation to a thermal DQPT, where the initial thermal density operator remains intact, by means of such transformations.

DQPT is not only a theoretical concept. A number of articles have already presented the experimental observations at zero temperature, following the theoretical predictions. See e.g. [22], [11], which are also reviewed in [15, Section 4]. A brief summary of experiments of DQPT is given in the recent paper [19]. Though we do not find any experimental result treating temperature as a control parameter of DQPT, the authors of [17] argue that their finite-temperature formalism of DQPT reproduces the experimental observation of [11], because the experiment is “unavoidably performed on mixed states”.

Here we add one remark that our notion of phase diagram is different from the dynamical phase diagram defined in the physics literature (e.g. [46], [14], [31], [39]).

Our phase diagram drawn in [25, Subsection 2.1] shows the boundary of a region where the gap equation has a positive solution in the plane of (inverse temperature, real time). On the other hand, the dynamical phase diagrams in [46], [14], [31], [39] show boundaries of different regions in a plane of 2 parameters, which does not include the real time variable. The 2 parameters plus the real time variable control the dynamical analogue of free energy density whose singularity with the time variable defines DQPT. The 2 parameters belong to the inside of the boundaries if the DQPT occurs, i.e. the dynamical free energy density is non-analytic with the time variable.

In [25, Section 2] we proved that the phase transition driven by the real time variable is of 2nd order and that driven by the temperature is also of 2nd order at most of the critical temperatures. Recall that we define the order of phase transition in terms of regularity of the extended free energy density, which is an analogy to the Ehrenfest classification. Moreover we gave a necessary and sufficient condition for the representative phase boundary to have only one local minimum point (LMiP). More precisely, the condition is that the minimum of the modulus of the free dispersion relation over the maximum is larger than the critical value  $\sqrt{17 - 12\sqrt{2}}$ . We did not relate the order of the phase transition to the uniqueness of LMiP, though in [25, Remark 2.6] we mentioned a possibility of the temperature-driven phase transition of higher order in case where the phase boundary has a stationary point of inflection.

The main results of this paper are obtained by pursuing the question raised in [25, Remark 2.6]. Admitting the free energy density of the BCS model with imaginary magnetic field characterized in [25, Theorem 1.3 (ii)], we prove that we can choose a non-vanishing free dispersion relation and a weak coupling constant so that the system has a temperature-driven phase transition of order  $n$  for some  $n \in 4\mathbb{N} + 2$  ( $= \{6, 10, 14, \dots\}$ ) if and only if the minimum of the modulus of the free dispersion relation over the maximum is less than or equal to  $\sqrt{17 - 12\sqrt{2}}$ . We also prove equivalence between existence of a higher order phase transition (HOPT) driven by temperature and existence of a stationary point of inflection (SPI) on the phase boundary. It follows in particular that the temperature-driven phase transition is of order  $n \in 4\mathbb{N} + 2$  if the critical inverse temperature is a SPI of the phase boundary, it is of 2nd order otherwise. In the previous work [25] we were unaware of the relation between the order of the phase transition and the critical value  $\sqrt{17 - 12\sqrt{2}}$ . The essential new finding in this paper is that the universal constant  $\sqrt{17 - 12\sqrt{2}}$  is also a critical value for existence of a HOPT driven by temperature.

Once the equivalence between existence of a HOPT and existence of a SPI is established, we focus on the problem of existence / non-existence of a SPI. Our study on the uniqueness / non-uniqueness of a LMiP of the phase boundary in [25, Section 2] essentially helps us in this part. The proof of uniqueness of LMiP is technically close to the proof of non-existence of SPI. Specifically, we apply [25, Lemma 2.12] as the key lemma. When there are 2 LMiPs on the phase boundary, we can continuously transform the free dispersion relation until one of the LMiPs disappears. In the middle of this process a SPI appears on the phase boundary. This is how we prove the existence of a SPI and thus a HOPT. We remark that [25, Lemma 2.15] plays a key role in the proof of the existence in a critical case. After proving the main theorems we study specific models in terms of SPI and HOPT.

There we also apply [25, Lemma 2.24] and admit the proof of [25, Proposition 2.26]. The critical value  $\sqrt{17 - 12\sqrt{2}}$ , whose original meaning is a root of the polynomial  $X^4 - 34X^2 + 1$ , is already involved in [25, Lemma 2.12], [25, Lemma 2.15] and [25, Lemma 2.24]. This work can certainly be seen as a continuation of [25, Section 2] from the technical viewpoint.

As explained in the beginning, the main reason for focusing on non-vanishing free dispersion relations is that the derivation of the free energy density is justified for wide range of parameters. It is encouraging that this class of free dispersion relations cover benchmark models showing DQPTs at positive temperature, namely Fermionic Hamiltonians for topological insulator. Let  $H_0, H$  be gapped Hamiltonians with different ground state topology in (1.3). It has been vigorously studied if such a system exhibits DQPT in recent years. Though the benchmark models are spinless, they can be written with single-particle Hamiltonian matrices belonging to our class. They are e.g. the Haldane model (2-dimensional, 2-band, [13], [17]), the Su-Schrieffer-Heeger (SSH) model (1-dimensional, 2-band, [36], [19]). Though it is related to DQPT at zero temperature, the paper [32] introduced a multi-band version of the SSH model, which belongs to our class as well. We will show how to construct the Haldane model and the SSH model in Remark 1.2 as concrete examples of our free Hamiltonian.

No physical interpretation has been given to non-analyticity of the functions

$$\beta \mapsto \lim_{N \rightarrow \infty} \frac{1}{N} \log \left( \frac{\text{Tr}(e^{-\beta H_0} e^{-itH})}{\text{Tr } e^{-\beta H_0}} \right), \quad \beta \mapsto \lim_{N \rightarrow \infty} \frac{1}{N} \log \left( \frac{\text{Tr}(e^{-\beta H_0} e^{-itH_0} e^{itH_1})}{\text{Tr } e^{-\beta H_0}} \right)$$

in the context of DQPT as far as the author knows. Therefore, what this paper presents as the main results are novel mathematical properties of the BCS model, rather than physical properties which can be immediately interpreted in terms of DQPT at present. One interesting aspect of our DQPT is that the dynamical free energy density (1.5) is equal to the minimum of a function whose minimizer is the order parameter solving the gap equation. It is actually written as the right-hand side of (1.7). Whether one can construct an analogue of the Landau theory of EPT in the context of DQPT is posed in [16] as one open question. The paper [38] presents such a trial in the transverse-field Ising chain. Since there is a notable structural resemblance to the conventional macroscopic theory of EPT, it is a natural mathematical interest to pursue the analogy by studying the degree of non-analyticity of our free energy density with  $\beta$ . Concerning the conventional BCS model without imaginary magnetic field, it is a general consensus that the temperature-driven transition between superconducting / normal phase is of 2nd order. Despite that there are many mathematical papers studying the BCS theory (see e.g. the review articles [12], [4]), it seems that only a few have tried to prove the order of the phase transition. There are mathematical constructions toward the 2nd order phase transition in a BCS-type thermodynamic potential by Watanabe ([41], [42], [43], [44], [45]).

We find more articles related to the present paper's theme, namely HOPT in superconductors, in physics literature. Cronström and Noga [5] obtained a mean field solution to the BCS model in thin films and a layered structure, which shows a 3rd order superconducting phase transition. There are attempts to explain experimentally observed anomalous superconducting phase transitions in terms of HOPT, especially of 3rd / 4th order, by extending the phenomenological Ginzburg-Landau theory. Kumar and the coauthors ([27], [29], [30], [28], [10]) initiated this

approach. Later Ekuma and the coauthors ([6], [7], [9], [8]) continued in this line of research, aiming in particular to explain a 3rd order phase transition in iron-based superconductors.

This paper is organized as follows. In the rest of this section we prepare necessary concepts and state the main results of this paper. In Section 2 we prove the main theorems step by step by establishing various propositions ranging from the equivalence between HOPT and SPI to existence / non-existence of a SPI. In Section 3 we study whether HOPT is possible in multi-orbital non-hopping models and a one-dimensional nearest-neighbor hopping model. These are the same models as those analyzed in [25, Subsection 2.3] with regard to uniqueness / non-uniqueness of a LMIP of the phase boundary.

## 1.2 The main results

We keep using many of the notations introduced in [25, Section 1, Section 2]. Let us reintroduce the important ones for clarity of the present paper. With the dimension  $d \in \mathbb{N}$  let  $(\hat{\mathbf{v}}_j)_{j=1}^d$  denote a basis of  $\mathbb{R}^d$ . Define the subset  $\Gamma_\infty^*$  of  $\mathbb{R}^d$  by

$$\Gamma_\infty^* := \left\{ \sum_{j=1}^d \hat{k}_j \hat{\mathbf{v}}_j \mid \hat{k}_j \in [0, 2\pi] \ (j = 1, \dots, d) \right\}.$$

Originally the set  $\Gamma_\infty^*$  is the continuum limit of a finite momentum lattice spanned by  $(\hat{\mathbf{v}}_j)_{j=1}^d$ , which is denoted by  $\Gamma^*$  below. Take  $b \in \mathbb{N}$  and  $e_{min}, e_{max} \in \mathbb{R}_{>0}$  satisfying  $e_{min} \leq e_{max}$ . The set  $\mathcal{E}(e_{min}, e_{max})$  of one-particle Hamiltonians in momentum space is defined as follows.  $E \in \mathcal{E}(e_{min}, e_{max})$  if and only if

$$\begin{aligned} (1.6) \quad & E \in C^\infty(\mathbb{R}^d, \text{Mat}(b, \mathbb{C})), \\ & E(\mathbf{k}) = E(\mathbf{k})^*, \quad \forall \mathbf{k} \in \mathbb{R}^d, \\ & E(\mathbf{k} + 2\pi \hat{\mathbf{v}}_j) = E(\mathbf{k}), \quad \forall \mathbf{k} \in \mathbb{R}^d, \quad j \in \{1, \dots, d\}, \\ & E(\mathbf{k}) = \overline{E(-\mathbf{k})}, \quad \forall \mathbf{k} \in \mathbb{R}^d, \\ & \inf_{\mathbf{k} \in \mathbb{R}^d} \inf_{\substack{\mathbf{u} \in \mathbb{C}^b \\ \text{with } \|\mathbf{u}\|_{\mathbb{C}^b} = 1}} \|E(\mathbf{k})\mathbf{u}\|_{\mathbb{C}^b} = e_{min} (> 0), \\ & \sup_{\mathbf{k} \in \mathbb{R}^d} \|E(\mathbf{k})\|_{b \times b} = e_{max}. \end{aligned}$$

Here  $\text{Mat}(b, \mathbb{C})$  is the complex Banach space of  $b \times b$  complex matrices equipped with the operator norm  $\|\cdot\|_{b \times b}$ . Also,  $\|\cdot\|_{\mathbb{C}^b}$  denotes the canonical norm of  $\mathbb{C}^b$  induced by the Hermitian inner product.

Some of the properties assumed in  $\mathcal{E}(e_{min}, e_{max})$  will not be used in this paper at all. For example, we do not need to assume that  $\mathbf{k} \mapsto E(\mathbf{k})$  is infinitely differentiable and (1.6) to complete the proofs of the main results. We keep these conditions in this paper in order to emphasize that the free energy density analyzed in this paper is the same as that rigorously derived in [25, Theorem 1.3 (ii)] by assuming these conditions.

Our main theorems concern the free energy density which explicitly involves the solution  $\Delta$  to the gap equation. Therefore we have to introduce the gap equation in advance. For  $E \in \mathcal{E}(e_{min}, e_{max})$  the function  $g_E : \mathbb{R}_{>0} \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  is defined by

$$g_E(x, t, z)$$

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

$$D_d := |\det(\hat{\mathbf{v}}_1, \dots, \hat{\mathbf{v}}_d)|^{-1} (2\pi)^{-d}.$$

The parameter  $U$  is real, negative and called coupling constant. Remind us that for any function  $f : \mathbb{R} \setminus \{0\} \rightarrow \mathbb{C}$  and  $\mathbf{k} \in \mathbb{R}^d$   $f(E(\mathbf{k})) (\in \operatorname{Mat}(b, \mathbb{C}))$  is defined via the spectral decomposition of  $E(\mathbf{k})$ . The next lemma is essentially the same as [25, Lemma 1.1].

**Lemma 1.1.** *The following statements hold for any  $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$ . The equation  $g_E(\beta, t, \Delta) = 0$  has a solution  $\Delta$  in  $[0, \infty)$  if and only if  $g_E(\beta, t, 0) \geq 0$ . Moreover, if a solution exists in  $[0, \infty)$ , it is unique.*

This lemma enables us to define the function  $\Delta : \mathbb{R}_{>0} \times \mathbb{R} \rightarrow \mathbb{R}_{\geq 0}$  as follows. For  $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$ , if  $g_E(\beta, t, 0) \geq 0$ , let  $\Delta(\beta, t) \in \mathbb{R}_{\geq 0}$  be such that  $g_E(\beta, t, \Delta(\beta, t)) = 0$ . If  $g_E(\beta, t, 0) < 0$ , let  $\Delta(\beta, t) := 0$ . Observe that

$$\Delta(\beta, t) = \Delta(\beta, \delta t + 4\pi m), \quad \forall (\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}, \quad \delta \in \{1, -1\}, \quad m \in \mathbb{Z}.$$

Moreover, we define the function  $F_E : \mathbb{R}_{>0} \times \mathbb{R} \rightarrow \mathbb{R}$  by

$$(1.7) \quad F_E(\beta, t) := \frac{\Delta(\beta, t)^2}{|U|} - \frac{D_d}{\beta} \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr} \log \left( 2 \cos \left( \frac{t}{2} \right) e^{-\beta E(\mathbf{k})} + e^{\beta(\sqrt{E(\mathbf{k})^2 + \Delta(\beta, t)^2} - E(\mathbf{k}))} + e^{-\beta(\sqrt{E(\mathbf{k})^2 + \Delta(\beta, t)^2} + E(\mathbf{k}))} \right).$$

We can see that

$$(1.8) \quad F_E(\beta, t) = F_E(\beta, \delta t + 4\pi m), \quad \forall (\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}, \quad \delta \in \{1, -1\}, \quad m \in \mathbb{Z}.$$

According to [25, Theorem 1.3 (ii)], for any  $E \in \mathcal{E}(e_{\min}, e_{\max})$  there exists  $c' \in (0, 1]$  such that for any  $\beta \in \mathbb{R}_{>0}$ ,  $t \in \mathbb{R}$ ,

$$(1.9) \quad U \in \left( -\frac{2c'}{b} \min\{e_{\min}, e_{\min}^{d+1}\}, 0 \right),$$

$$F_E(\beta, t) = \lim_{\substack{L \rightarrow \infty \\ L \in \mathbb{N}}} \left( -\frac{1}{\beta L^d} \log (\operatorname{Tr} e^{-\beta \mathbf{H} + it \mathbf{S}_z}) \right),$$

where  $c'$  depends only on  $d, b, (\hat{\mathbf{v}}_j)_{j=1}^d$  and the quantity

$$(1.10) \quad \sup_{\mathbf{k} \in \mathbb{R}^d} \sup_{\substack{m_j \in \mathbb{N} \cup \{0\} \\ (j=1, \dots, d)}} \left\| \prod_{j=1}^d \frac{\partial^{m_j}}{\partial k_j^{m_j}} E(\mathbf{k}) \right\|_{b \times b} 1_{\sum_{j=1}^d m_j \leq d+2}.$$

For any proposition  $P$   $1_P := 1$  if  $P$  is true,  $1_P := 0$  otherwise. The operator  $\mathbf{H}$  is the BCS model with the reduced quartic interaction and the one-particle Hamiltonian  $E(\cdot)$ , and  $\mathbf{S}_z$  is the  $z$ -component of the spin operator. The negative parameter  $U$

controls the strength of attractive interaction between Cooper pairs in the BCS model  $\mathsf{H}$ . More precisely,

$$\begin{aligned}\mathsf{H} &:= \frac{1}{L^d} \sum_{(\rho, \mathbf{x}), (\eta, \mathbf{y}) \in \mathcal{B} \times \Gamma} \sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{\mathbf{k} \in \Gamma^*} e^{i\langle \mathbf{x} - \mathbf{y}, \mathbf{k} \rangle} E(\mathbf{k})(\rho, \eta) \psi_{\rho \mathbf{x} \sigma}^* \psi_{\eta \mathbf{y} \sigma} \\ &\quad + \frac{U}{L^d} \sum_{(\rho, \mathbf{x}), (\eta, \mathbf{y}) \in \mathcal{B} \times \Gamma} \psi_{\rho \mathbf{x} \uparrow}^* \psi_{\rho \mathbf{x} \downarrow}^* \psi_{\eta \mathbf{y} \downarrow} \psi_{\eta \mathbf{y} \uparrow}, \\ \mathsf{S}_z &:= \frac{1}{2} \sum_{(\rho, \mathbf{x}) \in \mathcal{B} \times \Gamma} (\psi_{\rho \mathbf{x} \uparrow}^* \psi_{\rho \mathbf{x} \uparrow} - \psi_{\rho \mathbf{x} \downarrow}^* \psi_{\rho \mathbf{x} \downarrow}),\end{aligned}$$

where  $\mathcal{B} := \{1, 2, \dots, b\}$ ,

$$\begin{aligned}\Gamma &:= \left\{ \sum_{j=1}^d m_j \mathbf{v}_j \mid m_j \in \{0, 1, \dots, L-1\} \ (j = 1, \dots, d) \right\}, \\ \Gamma^* &:= \left\{ \sum_{j=1}^d \hat{m}_j \hat{\mathbf{v}}_j \mid \hat{m}_j \in \left\{0, \frac{2\pi}{L}, \frac{4\pi}{L}, \dots, 2\pi - \frac{2\pi}{L}\right\} \ (j = 1, \dots, d) \right\},\end{aligned}$$

$(\mathbf{v}_j)_{j=1}^d$  is a basis of  $\mathbb{R}^d$ , dual to  $(\hat{\mathbf{v}}_j)_{j=1}^d$  and for  $(\rho, \mathbf{x}, \sigma) \in \mathcal{B} \times \Gamma \times \{\uparrow, \downarrow\}$   $\psi_{\rho \mathbf{x} \sigma}$  ( $\psi_{\rho \mathbf{x} \sigma}^*$ ) is the annihilation (creation) operator on the Fermionic Fock space  $F_f(L^2(\mathcal{B} \times \Gamma \times \{\uparrow, \downarrow\}))$ . The Fermionic operators appear only in this section. As we want to relate the present construction to the original definitions,  $U$  is taken as a negative parameter throughout this paper even though we essentially deal with  $|U|$  in every estimate.

Here we remark for clarity that [25, Theorem 1.3] is claimed for  $t = -\beta\theta$  with any  $\theta \in \mathbb{R}$ . The arbitrariness of  $\theta$  ensures that [25, Theorem 1.3 (ii)] is equivalent to the above statement.

**Remark 1.2.** We can formulate various free Hamiltonians into the form

$$\frac{1}{L^d} \sum_{(\rho, \mathbf{x}), (\eta, \mathbf{y}) \in \mathcal{B} \times \Gamma} \sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{\mathbf{k} \in \Gamma^*} e^{i\langle \mathbf{x} - \mathbf{y}, \mathbf{k} \rangle} E(\mathbf{k})(\rho, \eta) \psi_{\rho \mathbf{x} \sigma}^* \psi_{\eta \mathbf{y} \sigma}$$

with  $E \in \mathcal{E}(e_{\min}, e_{\max})$ . The most standard one is the nearest-neighbor hopping model on the (hyper-)cubic lattice

$$(1.11) \quad E(\mathbf{k}) = 2 \sum_{j=1}^d \cos k_j - \mu, \quad \mathbf{k} \in \mathbb{R}^d$$

with  $\mu \in \mathbb{R} \setminus [-2d, 2d]$ . In this case  $b = 1$ ,  $(\mathbf{v}_j)_{j=1}^d$ ,  $(\hat{\mathbf{v}}_j)_{j=1}^d$  are the canonical bases of  $\mathbb{R}^d$  and  $e_{\min} = |\mu| - 2d (> 0)$ ,  $e_{\max} = |\mu| + 2d$ . In the following we present a couple of benchmark models studied in the context of DQPT at finite temperature. We note, however, that these models are supposed to describe spinless Fermions in the papers we refer to.

**The Su-Schrieffer-Heeger (SSH) model** The SSH model describes a 1-dimensional, 2-band insulator. It was originally proposed as a model of

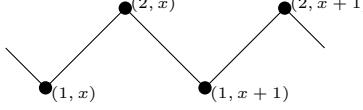


Figure 1: The lattice for the SSH model.

polyacetylene ([36]). It was analyzed in [19] to display DQPT at finite temperature. To formulate the model, we set  $b = 2$ . The spatial lattice is identified as  $\{1, 2\} \times \mathbb{Z}$ . In our finite-volume formulation  $\Gamma = \{0, 1, \dots, L-1\}$ ,  $\Gamma^* = \{0, \frac{2\pi}{L}, \dots, \frac{2\pi}{L}(L-1)\}$ . The lattice linked by the nearest-neighbor hopping is pictured in Figure 1.

The corresponding one-particle Hamiltonian matrix  $E$  is defined by

$$E(k) = \begin{pmatrix} 0 & J_1 + J_2 e^{-ik} \\ J_1 + J_2 e^{ik} & 0 \end{pmatrix}, \quad k \in \mathbb{R},$$

where  $J_1, J_2 (\in \mathbb{R})$  are hopping amplitude. Set

$$f(k) := \sqrt{J_1^2 + 2 \cos k J_1 J_2 + J_2^2}$$

for  $k \in \mathbb{R}$ . Since the eigenvalues of  $E(k)$  are  $\pm f(k)$ ,

$$\begin{aligned} \inf_{k \in \mathbb{R}} \inf_{\substack{\mathbf{u} \in \mathbb{C}^2 \\ \text{with } \|\mathbf{u}\|_{\mathbb{C}^2} = 1}} \|E(k)\mathbf{u}\|_{\mathbb{C}^2} &= \min_{k \in \mathbb{R}} f(k) = ||J_1| - |J_2||, \\ \sup_{k \in \mathbb{R}} \|E(k)\|_{2 \times 2} &= \max_{k \in \mathbb{R}} f(k) = |J_1| + |J_2|. \end{aligned}$$

Thus if  $|J_1| \neq |J_2|$ ,  $E \in \mathcal{E}(e_{\min}, e_{\max})$  with  $e_{\min} = ||J_1| - |J_2|| (> 0)$ ,  $e_{\max} = |J_1| + |J_2|$ .

**The Haldane model** Let  $b = 2$ ,  $\mathbf{v}_1 = (1, 0)^T$ ,  $\mathbf{v}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})^T$ ,  $\hat{\mathbf{v}}_1 = (1, -\frac{1}{\sqrt{3}})^T$ ,  $\hat{\mathbf{v}}_2 = (0, \frac{2}{\sqrt{3}})^T$ . The vectors  $\mathbf{v}_1, \mathbf{v}_2$  form a basis of  $\mathbb{R}^2$  and  $(\hat{\mathbf{v}}_j)_{j=1}^2$  is its dual basis. The honeycomb lattice is expressed as

$$\{1, 2\} \times \{m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2 \mid m_1, m_2 \in \mathbb{Z}\}.$$

In the Haldane model ([13]) not only the nearest-neighbor hopping but also the next-nearest-neighbor hopping is considered. The honeycomb lattice linked by these hoppings is pictured in Figure 2. See [21] for experimental realization of the model.

A version of the Haldane model studied in [17] can be formulated with

$$\begin{aligned} E(\mathbf{k}) &= (E(\mathbf{k})(\rho, \eta))_{1 \leq \rho, \eta \leq 2}, \\ E(\mathbf{k})(1, 1) &= m - 2J'(\cos(\langle \mathbf{k}, \mathbf{v}_1 - \mathbf{v}_2 \rangle) + \cos(\langle \mathbf{k}, \mathbf{v}_1 \rangle) + \cos(\langle \mathbf{k}, \mathbf{v}_2 \rangle)), \\ E(\mathbf{k})(1, 2) &= J(1 + e^{-i\langle \mathbf{k}, \mathbf{v}_1 \rangle} + e^{-i\langle \mathbf{k}, \mathbf{v}_2 \rangle}), \\ E(\mathbf{k})(2, 1) &= J(1 + e^{i\langle \mathbf{k}, \mathbf{v}_1 \rangle} + e^{i\langle \mathbf{k}, \mathbf{v}_2 \rangle}), \\ E(\mathbf{k})(2, 2) &= -m + 2J'(\cos(\langle \mathbf{k}, \mathbf{v}_1 - \mathbf{v}_2 \rangle) + \cos(\langle \mathbf{k}, \mathbf{v}_1 \rangle) + \cos(\langle \mathbf{k}, \mathbf{v}_2 \rangle)), \end{aligned}$$

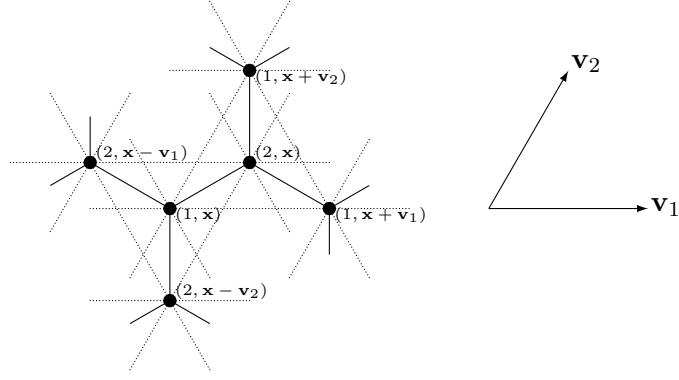


Figure 2: The honeycomb lattice linked by the nearest-neighbor hopping (solid lines) and the next-nearest-neighbor hopping (dashed lines).

where  $J(\in \mathbb{R} \setminus \{0\})$ ,  $J'(\in \mathbb{R})$  is the nearest-neighbor, the next-nearest-neighbor hopping amplitude respectively and  $m(\in \mathbb{R})$  is the on-site energy. It is clear that all the conditions of  $\mathcal{E}(e_{\min}, e_{\max})$  except for the spectral properties are satisfied. Set

$$g(\hat{k}_1, \hat{k}_2) := ((m - 2J'(\cos(\hat{k}_1 - \hat{k}_2) + \cos \hat{k}_1 + \cos \hat{k}_2))^2 + J^2(1 + \cos \hat{k}_1 + \cos \hat{k}_2)^2 + J^2(\sin \hat{k}_1 + \sin \hat{k}_2)^2)^{\frac{1}{2}}.$$

A direct calculation shows that the eigenvalues of  $E(\hat{k}_1 \hat{\mathbf{v}}_1 + \hat{k}_2 \hat{\mathbf{v}}_2)$  ( $\hat{k}_1, \hat{k}_2 \in \mathbb{R}$ ) are  $\pm g(\hat{k}_1, \hat{k}_2)$ . Let us determine  $\min_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2)$ ,  $\max_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2)$  exactly. Observe that

$$g(k_1, k_2) = ((m - 2J'h(k_1, k_2))^2 + J^2(3 + 2h(k_1, k_2)))^{\frac{1}{2}},$$

where  $h(k_1, k_2) := \cos(k_1 - k_2) + \cos k_1 + \cos k_2$ . Moreover,

$$\begin{aligned} \max_{k_1, k_2 \in \mathbb{R}} h(k_1, k_2) &= 3, \\ \min_{k_1, k_2 \in \mathbb{R}} h(k_1, k_2) &= \min_{k_1, k_2 \in \mathbb{R}} (\operatorname{Re}(e^{ik_1}(e^{-ik_2} + 1)) + \cos k_2) \\ &= \min_{k_2 \in \mathbb{R}} (-|e^{-ik_2} + 1| + \cos k_2) = -\frac{3}{2}. \end{aligned}$$

Thus it suffices to find the minimum and the maximum of the function

$$x \mapsto ((m - 2J'x)^2 + J^2(3 + 2x))^{\frac{1}{2}}$$

in  $[-\frac{3}{2}, 3]$ . We can find them in each of the cases  $J' = 0$ ,  $J' \neq 0$  and  $\frac{2mJ' - J^2}{4J'^2} < -\frac{3}{2}$ ,  $J' \neq 0$  and  $-\frac{3}{2} \leq \frac{2mJ' - J^2}{4J'^2} \leq 3$ ,  $J' \neq 0$  and  $\frac{2mJ' - J^2}{4J'^2} > 3$ . The results are organized as follows.

- If  $J^2 < 2J'(m - 6J')$ ,

$$\min_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) = \sqrt{(m - 6J')^2 + 9J^2}, \quad \max_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) = |m + 3J'|.$$

- If  $2J'(m - 6J') \leq J^2 \leq 2J'(m + 3J')$ ,

$$\min_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) = \frac{|J|}{2|J'|} \sqrt{4J'(m + 3J') - J^2},$$

$$\max_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) = \max \left\{ |m + 3J'|, \sqrt{(m - 6J')^2 + 9J^2} \right\}.$$

- If  $J^2 > 2J'(m + 3J')$ ,

$$\min_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) = |m + 3J'|, \quad \max_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) = \sqrt{(m - 6J')^2 + 9J^2}.$$

We can deduce from above that  $\min_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2) > 0$  for any  $J \in \mathbb{R} \setminus \{0\}$  if and only if  $m + 3J' \neq 0$ . Therefore on the assumption that  $J \in \mathbb{R} \setminus \{0\}$  and  $m + 3J' \neq 0$   $E \in \mathcal{E}(e_{\min}, e_{\max})$  with  $e_{\min} = \min_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2)$ ,  $e_{\max} = \max_{k_1, k_2 \in \mathbb{R}} g(k_1, k_2)$ .

Next let us recall the notion of phase boundary. We define the subsets  $Q_+$ ,  $Q_-$ ,  $Q_0$  of  $\mathbb{R}_{>0} \times \mathbb{R}$  by

$$\begin{aligned} Q_+ &:= \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid g_E(\beta, t, 0) > 0\}, \\ Q_- &:= \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid g_E(\beta, t, 0) < 0\}, \\ Q_0 &:= \{(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R} \mid g_E(\beta, t, 0) = 0\}. \end{aligned}$$

It follows that  $\mathbb{R}_{>0} \times \mathbb{R} = Q_+ \sqcup Q_- \sqcup Q_0$  and  $\Delta(\beta, t) > 0$  if and only if  $(\beta, t) \in Q_+$ . We call  $Q_0$  phase boundary. The main theme of this paper is to study the regularity of  $F_E$  on the phase boundary  $Q_0$ . Because of the periodicity of  $g_E(\beta, t, 0)$  with  $t$ ,  $Q_0$  is infinite union of copies of one representative curve. This paper's main problems can be solved by focusing on the representative curve. The next lemma is essentially the same as [25, Lemma 1.2] and supports the well-definedness of the representative curve.

**Lemma 1.3.** *Assume that  $|U| < \frac{2e_{\min}}{b}$ . 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

$$\begin{aligned} g_E(\beta, \pi, 0) &< 0, \quad \forall \beta \in \mathbb{R}_{>0}, \\ g_E(\beta, 2\pi, 0) &> 0, \quad \forall \beta \in (0, \beta_c), \\ g_E(\beta_c, 2\pi, 0) &= 0, \\ g_E(\beta, 2\pi, 0) &< 0, \quad \forall \beta \in (\beta_c, \infty), \end{aligned}$$

where  $\tanh^{-1} : (-1, 1) \rightarrow \mathbb{R}$  is the inverse function of  $\tanh$ .

From here we always assume that  $U \in (-\frac{2e_{\min}}{b}, 0)$  so that the existence of the critical inverse temperature  $\beta_c$  is guaranteed by Lemma 1.3. By the monotone increasing property of  $t \mapsto g_E(\beta, t, 0)$  in  $(\pi, 2\pi)$  for any  $\beta \in (0, \beta_c)$  there uniquely exists  $\tau(\beta) \in (\pi, 2\pi)$  such that  $g_E(\beta, \tau(\beta), 0) = 0$ . This defines the function  $\tau : (0, \beta_c) \rightarrow (\pi, 2\pi)$ . By [25, Lemma 2.2 (i)]  $\tau \in C^\omega((0, \beta_c))$ . Remind us that for any open set  $O \subset \mathbb{R}^n$   $C^\omega(O)$  denotes the set of real analytic functions on  $O$ . Using the function  $\tau$ , we can characterize the phase boundary  $Q_0$  as follows.

$$\begin{aligned} (1.12) \quad Q_0 = & \{(\beta, \delta\tau(\beta) + 4\pi m) \mid \beta \in (0, \beta_c), \delta \in \{1, -1\}, m \in \mathbb{Z}\} \\ & \cup \{(\beta_c, 2\pi + 4\pi m) \mid m \in \mathbb{Z}\}. \end{aligned}$$

The above characterization was given in [25, (2.3)]. We can see that  $Q_0$  is a union of copies of

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

and thus we can consider the above set as the representative curve of the phase boundary. Moreover,

$$(1.13) \quad \begin{aligned} Q_+ &= \bigsqcup_{m \in \mathbb{Z}} \left\{ (\beta, t) \mid \beta \in (0, \beta_c), t \in (\tau(\beta) + 4\pi m, -\tau(\beta) + 4\pi(m+1)) \right\}, \\ Q_- &= \bigsqcup_{m \in \mathbb{Z}} \left\{ (\beta, t) \mid \beta \in (0, \beta_c), t \in (-\tau(\beta) + 4\pi m, \tau(\beta) + 4\pi m) \right\} \sqcup (\beta_c, \infty) \times \mathbb{R}. \end{aligned}$$

This interestingly suggests that in this weak coupling regime the gap equation has a positive solution only when the temperature is high.

To state the main theorems, we have to make clear our definition of phase transition. For  $(\rho, \eta) = (+, -)$  or  $(-, +)$  let us set

$$Q_{\rho, \eta} := \left\{ (\beta_0, t_0) \in Q_0 \mid \exists \varepsilon \in \mathbb{R}_{>0} \text{ s.t. } \begin{array}{l} (\beta, t_0) \in Q_\rho, \forall \beta \in (\beta_0 - \varepsilon, \beta_0), \\ (\beta, t_0) \in Q_\eta, \forall \beta \in (\beta_0, \beta_0 + \varepsilon). \end{array} \right\}.$$

Here we should recall the fact that for any  $E \in \mathcal{E}(e_{\min}, e_{\max})$

$$(1.14) \quad F_E|_{Q_+ \cup Q_-} \in C^\omega(Q_+ \cup Q_-), \quad F_E \in C^1(\mathbb{R}_{>0} \times \mathbb{R}),$$

which was proved in [25, Proposition 2.5 (i)]. For  $(\beta_0, t_0) \in \mathbb{R}_{>0} \times \mathbb{R}$ ,  $n \in \mathbb{N}(\{1, 2, 3, \dots\})$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$  we define the properties  $(\text{PT})_{n,(\rho,\eta)}(\beta_0, t_0)$ ,  $(\text{PT})_{n,(\rho,\eta)}$  as follows.

$$\begin{aligned} &(\text{PT})_{n,(\rho,\eta)}(\beta_0, t_0) \\ &(\beta_0, t_0) \in Q_{\rho, \eta}, \\ &\lim_{\beta \nearrow \beta_0} \frac{\partial^m F_E}{\partial \beta^m}(\beta, t_0), \lim_{\beta \searrow \beta_0} \frac{\partial^m F_E}{\partial \beta^m}(\beta, t_0) \text{ converge to finite values} \\ &\text{for any } m \in \{0, 1, \dots, n\}, \text{ and} \\ &\lim_{\beta \nearrow \beta_0} \frac{\partial^m F_E}{\partial \beta^m}(\beta, t_0) = \lim_{\beta \searrow \beta_0} \frac{\partial^m F_E}{\partial \beta^m}(\beta, t_0), \forall m \in \{0, 1, \dots, n-1\}, \\ &\lim_{\beta \nearrow \beta_0} \frac{\partial^n F_E}{\partial \beta^n}(\beta, t_0) \neq \lim_{\beta \searrow \beta_0} \frac{\partial^n F_E}{\partial \beta^n}(\beta, t_0). \end{aligned}$$

$$(\text{PT})_{n,(\rho,\eta)} \quad \text{There exists } (\beta_0, t_0) \in \mathbb{R}_{>0} \times \mathbb{R} \text{ such that } (\text{PT})_{n,(\rho,\eta)}(\beta_0, t_0) \text{ holds.}$$

By analogy with the Ehrenfest classification we state that the system has a phase transition of order  $n$  driven by temperature when  $(\text{PT})_{n,(\rho,\eta)}$  holds. According to [25, Proposition 2.5 (ii)],  $(\text{PT})_{2,(+,-)}$ ,  $(\text{PT})_{2,(-,+)}$  hold for any  $e_{\min}, e_{\max} \in \mathbb{R}_{>0}$  satisfying  $e_{\min} \leq e_{\max}$ ,  $U \in (-\frac{2e_{\min}}{b}, 0)$  and  $E \in \mathcal{E}(e_{\min}, e_{\max})$ . The question here is whether  $(\text{PT})_{n,(\rho,\eta)}$  holds for  $n \geq 3$ , or in other words, a phase transition of order  $n(\geq 3)$  driven by temperature occurs. The following fact based on (1.8), (1.12), (1.13) will be useful later.

**Lemma 1.4.** Let  $\beta_0 \in (0, \beta_c]$ ,  $n \in \mathbb{N}$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$ . The following statements are equivalent to each other.

- There exists  $t_0 \in \mathbb{R}$  such that  $(PT)_{n,(\rho,\eta)}(\beta_0, t_0)$  holds.
- $\{t \in \mathbb{R} \mid (\beta_0, t) \in Q_{\rho,\eta}\} \neq \emptyset$  and for any  $t_0 \in \mathbb{R}$  satisfying  $(\beta_0, t_0) \in Q_{\rho,\eta}$   $(PT)_{n,(\rho,\eta)}(\beta_0, t_0)$  holds.
- If  $\beta_0 < \beta_c$ ,  $(PT)_{n,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  holds. If  $\beta_0 = \beta_c$ ,  $(PT)_{n,(\rho,\eta)}(\beta_0, 2\pi)$  holds.

In addition, we need to prepare the concept of stationary point of inflection (SPI).

**Definition 1.5.** Let  $a, b, c \in \mathbb{R}$  satisfy  $a < c < b$ . Let  $f \in C^1((a, b), \mathbb{R})$ .

(1) We call  $c$  rising stationary point of inflection of  $f$  if there exists  $\varepsilon \in \mathbb{R}_{>0}$  such that

$$\begin{aligned} (c - \varepsilon, c + \varepsilon) &\subset (a, b), \\ \frac{df}{dx}(c) &= 0, \\ \frac{df}{dx}(x) &> 0, \quad \forall x \in (c - \varepsilon, c + \varepsilon) \setminus \{c\}. \end{aligned}$$

(2) We call  $c$  falling stationary point of inflection of  $f$  if there exists  $\varepsilon \in \mathbb{R}_{>0}$  such that

$$\begin{aligned} (c - \varepsilon, c + \varepsilon) &\subset (a, b), \\ \frac{df}{dx}(c) &= 0, \\ \frac{df}{dx}(x) &< 0, \quad \forall x \in (c - \varepsilon, c + \varepsilon) \setminus \{c\}. \end{aligned}$$

(3) We call  $c$  stationary point of inflection of  $f$  if  $c$  is either a rising stationary point of inflection or a falling stationary point of inflection of  $f$ .

We define the properties  $(SPI)_\xi(\beta_0)$ ,  $(SPI)_\xi$  for  $\xi \in \{r, f\}$ ,  $\beta_0 \in \mathbb{R}_{>0}$  as follows.

$(SPI)_r(\beta_0)$   $\beta_0$  is a rising stationary point of inflection of  $\tau(\cdot) : (0, \beta_c) \rightarrow \mathbb{R}$ .  
 $(SPI)_f(\beta_0)$   $\beta_0$  is a falling stationary point of inflection of  $\tau(\cdot) : (0, \beta_c) \rightarrow \mathbb{R}$ .  
 $(SPI)_\xi$  There exists  $\beta_0 \in (0, \beta_c)$  such that  $(SPI)_\xi(\beta_0)$  holds.

Using these terms, we can state our main theorems. Theorem 1.6 summarizes the equivalence between existence of a HOPT and existence of a SPI plus the fact that if a HOPT occurs, it must be of order  $n \in 4\mathbb{N} + 2$ .

**Theorem 1.6.** Let  $d, b \in \mathbb{N}$ ,  $(\hat{\mathbf{v}}_j)_{j=1}^d$  be a basis of  $\mathbb{R}^d$ ,  $e_{\min}, e_{\max} \in \mathbb{R}_{>0}$  satisfy  $e_{\min} \leq e_{\max}$ ,  $U \in (-\frac{2e_{\min}}{b}, 0)$ ,  $E \in \mathcal{E}(e_{\min}, e_{\max})$ ,  $(\xi, \rho, \eta) \in \{(r, +, -), (f, -, +)\}$  and  $\beta_0 \in (0, \beta_c)$ . Then the following statements hold.

(i)  $(SPI)_\xi(\beta_0)$  holds if and only if there exists  $n \in 4\mathbb{N} + 2$  ( $= \{6, 10, 14, \dots\}$ ) such that  $(PT)_{n,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  holds.

- (ii)  $(SPI)_\xi$  does not hold if and only if  $(PT)_{2,(\rho,\eta)}(\beta, t)$  holds for any  $(\beta, t) \in Q_{\rho,\eta}$ .
- (iii)  $(\beta, t) \in Q_{\rho,\eta}$  and  $(PT)_{2,(\rho,\eta)}(\beta, t)$  does not hold if and only if there exists  $n \in 4\mathbb{N} + 2$  such that  $(PT)_{n,(\rho,\eta)}(\beta, t)$  holds.

In essence Theorem 1.7 gives a necessary and sufficient condition for existence of a HOPT and a SPI.

**Theorem 1.7.** *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  $e_{min} \leq e_{max}$  the following statements are equivalent to each other.*

- (i) *For any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$  there exist  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$ ,  $n \in 4\mathbb{N} + 2$  ( $= \{6, 10, 14, \dots\}$ ) such that  $(PT)_{n,(\rho,\eta)}$  holds.*
- (ii) *For any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $\xi \in \{r, f\}$  there exist  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$  such that  $(SPI)_\xi$  holds.*
- (iii)

$$\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}.$$

Theorem 1.7 is not logically equivalent to the following theorem, which essentially gives necessary and sufficient conditions for the temperature-driven phase transition to be of 2nd order.

**Theorem 1.8.** *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  $e_{min} \leq e_{max}$  the following statements are equivalent to each other.*

- (i) *There exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$ ,  $n \in \mathbb{N}_{\geq 3}$  ( $= \{3, 4, 5, \dots\}$ )  $(PT)_{n,(\rho,\eta)}$  does not hold.*
- (ii) *There exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$ ,  $(\beta, t) \in Q_{\rho,\eta}$   $(PT)_{2,(\rho,\eta)}(\beta, t)$  holds.*
- (iii) *There exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$ ,  $\xi \in \{r, f\}$   $(SPI)_\xi$  does not hold.*
- (iv)

$$\frac{e_{min}}{e_{max}} > \sqrt{17 - 12\sqrt{2}}.$$

**Remark 1.9.** Theorem 1.7 ensures existence of a HOPT and a SPI under the condition  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$ . One question is whether the HOPT and the SPI exist for the same  $U$  and  $E$ . In view of Theorem 1.6 (i), one can expect that they do. More precisely the following statement can be deduced from Theorem 1.7 and Corollary 2.5. Assume that  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$ . Then for any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $(\xi, \rho, \eta) \in \{(r, +, -), (f, -, +)\}$  there exist  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$ ,  $n \in 4\mathbb{N} + 2$  such that  $(PT)_{n,(\rho,\eta)}$  and  $(SPI)_\xi$  hold.

**Remark 1.10.** According to Theorem 1.7, a HOPT driven by temperature exists in the case  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$ . Strictly speaking, we cannot state that a HOPT exists in the BCS model with imaginary magnetic field unless the derivation of  $F_E(\beta, t)$  from the many-electron system is justified. In the case  $\frac{e_{min}}{e_{max}} < \sqrt{17 - 12\sqrt{2}}$  the existence of a HOPT is guaranteed while the derivation of  $F_E(\beta, t)$  is justified by [25, Theorem 1.3 (ii)]. See Remark 2.13. In the case  $\frac{e_{min}}{e_{max}} = \sqrt{17 - 12\sqrt{2}}$ , however, we cannot prove existence of a HOPT while justifying the derivation of  $F_E(\beta, t)$ . See Remark 2.16.

**Remark 1.11.** In Remark 1.2 we provided 3 models belonging to  $\mathcal{E}(e_{min}, e_{max})$  together with the explicit characterization of their  $e_{min}, e_{max}$ . We can apply Theorem 1.8 to conclude that if  $\frac{e_{min}}{e_{max}} > \sqrt{17 - 12\sqrt{2}}$  and the interaction is sufficiently small, there is no HOPT in the BCS model having one of these free Hamiltonians and the imaginary magnetic field. However, none of the above theorems implies existence of a HOPT in these models. In fact we do not have a general theory for existence of a HOPT when we vary  $e_{min}, e_{max}$  or other parameters inside a specific one-particle Hamiltonian matrix at present. We will consider this problem by focusing on a couple of simple models belonging to  $\mathcal{E}(e_{min}, e_{max})$  in Section 3.

Nevertheless we prove in Theorem 1.7 that if  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$ , there exists  $E \in \mathcal{E}(e_{min}, e_{max})$  such that a HOPT occurs with  $E$ . In this contradictory situation one might wonder how such  $E$  is characterized in the proof of Theorem 1.7. Here let us illustrate the corresponding part of the proof of Theorem 1.7. We will prove earlier in Corollary 2.5 that for  $(\xi, \rho, \eta) \in \{(r, +, -), (f, -, +)\}$   $(\text{SPI})_\xi$  holds if and only if  $(\text{PT})_{n,(\rho,\eta)}$  holds for some  $n \in 4\mathbb{N} + 2$ . Therefore if we find  $U \in (-\frac{2e_{min}}{b}, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$  such that a SPI exists, we can use the same pair  $(U, E)$  to prove existence of a HOPT. To prove existence of a SPI, we construct a family  $\{E_s\}_{s \in (0,1)} \subset \mathcal{E}(e_{min}, e_{max})$ . Each  $E_s$  can be written as  $E_s(\mathbf{k}) = \Phi_s(\mathbf{k})I_b$  ( $\mathbf{k} \in \mathbb{R}^d$ ) with the  $b \times b$  identity matrix  $I_b$  and a smooth real-valued function  $\Phi_s$ , which is parameterized by  $s$  and takes either  $e_{min}$  or  $e_{max}$  for most of  $\mathbf{k} \in \mathbb{R}^d$ . Then under the condition  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$  we prove existence of  $s \in (0, 1)$  and  $U$  such that a SPI exists for  $E_s$  and  $U$ , which implies existence of a HOPT as explained above. Here we emphasize that we essentially use the intermediate value theorem for a continuous function of  $s$  to prove existence of such  $s \in (0, 1)$  and we cannot determine it explicitly. In fact throughout this paper we are unable to exactly determine  $E \in \mathcal{E}(e_{min}, e_{max})$  for which a HOPT exists. When we prove HOPTs in a specific model in Section 3, not all the controlling parameters are made explicit.

**Remark 1.12.** Let us comment on whether we can extend the above results to gapless free dispersion relations. It is possible to extend the definition of our free energy density to include gapless dispersion relations. However, as explained in the beginning of the section, the domain of  $(\beta, t)$  where we can derive the free energy density from the many-Fermion system is severely restricted in the gapless case. Therefore it is difficult to give a coherent sense to our definition of phase transition as non-analyticity of the free energy density, which might not be the thermodynamic limit of a quantum many-body system. Putting the issue of derivation aside, one can analyze the free energy density itself in the whole domain of  $(\beta, t)$ . If the free Hamiltonian is gapless, the phase boundary is very different from that studied in this paper. In particular the order parameter  $\Delta(\beta, t)$  can be positive for any  $t \in \mathbb{R}$  in low temperatures. Remind us that  $\Delta(\beta, t) = 0$  for any  $t \in \mathbb{R}$  in low

temperatures in the present gapped case. This can be deduced as follows. Let us consider a gapless one-particle Hamiltonian matrix  $E$  satisfying that

$$\lim_{\beta \rightarrow \infty} D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr} \left( \frac{\tanh(\beta E(\mathbf{k}))}{E(\mathbf{k})} \right) = \infty.$$

For example the dispersion relation (1.11) with  $\mu \in (-2d, 2d)$  satisfies the above condition. Then there uniquely exists  $\hat{\beta} \in \mathbb{R}_{>0}$  such that

$$\begin{aligned} g_E(\hat{\beta}, 0, 0) &= -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr} \left( \frac{\tanh(\frac{\hat{\beta}}{2} E(\mathbf{k}))}{E(\mathbf{k})} \right) = 0, \\ g_E(\beta, 0, 0) &> 0, \quad \forall \beta \in (\hat{\beta}, \infty), \\ g_E(\beta, 0, 0) &< 0, \quad \forall \beta \in (0, \hat{\beta}). \end{aligned}$$

Therefore, for any  $(\beta, t) \in (\hat{\beta}, \infty) \times \mathbb{R}$   $g_E(\beta, t, 0) > 0$ , and thus there uniquely exists  $\Delta(\beta, t) \in \mathbb{R}_{>0}$  such that  $g_E(\beta, t, \Delta(\beta, t)) = 0$ . For  $\beta \in (0, \hat{\beta})$

$$\lim_{t \nearrow 2\pi} g_E(\beta, t, 0) = \infty,$$

which ensures that there uniquely exists  $\tau(\beta) \in (0, 2\pi)$  such that  $g_E(\beta, \tau(\beta), 0) = 0$ . We can conclude that the phase boundary exists only in  $(0, \hat{\beta}] \times \mathbb{R}$ . The same argument as in the proof of [25, Proposition 2.5 (iii)] implies that the phase transition driven by  $t$  is of 2nd order. Focusing on the subdomain  $(0, \hat{\beta}] \times \mathbb{R}$ , it seems possible to summarize the equivalence between existence of a HOPT and existence of a SPI in a way parallel to Theorem 1.6. Therefore it must suffice to find a SPI of the phase boundary to prove existence of a HOPT driven by  $\beta$ . However, to construct a gapless free dispersion relation with which the phase boundary has a SPI by modifying this paper's construction is not trivial. We wish to leave the (non-)existence theory of HOPT in the gapless case as an open problem without speculating more at this stage.

Concerning the standard dispersion relation (1.11), it is implied by Theorem 1.6 and Proposition 3.5 that if  $d = 1$  and  $|\mu| > 2$ , there is no HOPT. See [25, Remark 2.22] for deduction of this statement from Proposition 3.5. One interesting question is whether the same conclusion holds for any  $d \in \mathbb{N}$  and  $\mu \in \mathbb{R}$ , which covers the gapless case ( $|\mu| \leq 2d$ ). The question remains open at present.

**Remark 1.13.** In the series [23], [24], [25] the interaction is always the reduced BCS type

$$(1.15) \quad \frac{U}{L^d} \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} \psi_{\mathbf{x}\uparrow}^* \psi_{\mathbf{x}\downarrow}^* \psi_{\mathbf{y}\downarrow} \psi_{\mathbf{y}\uparrow}$$

with negative  $U$ , apart from the insertion of band index. It would be nice if we can derive the thermodynamic limit of the free energy density and analyze the nature of phase transition under the influence of imaginary magnetic field for more general interactions. However, it seems that interactions we can deal with in line with [23], [24], [25] are limited. Assume that  $\Gamma$  is spanned by the canonical basis  $(\mathbf{e}_j)_{j=1}^d$  for simplicity. We expect that if the interaction is of the form

$$(1.16) \quad U \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} v_L(\mathbf{x}, \mathbf{y}) \psi_{\mathbf{x}\uparrow}^* \psi_{\mathbf{x}\downarrow}^* \psi_{\mathbf{y}\downarrow} \psi_{\mathbf{y}\uparrow}$$

with a function  $v_L : \mathbb{Z}^d \times \mathbb{Z}^d \rightarrow \mathbb{R}_{\geq 0}$  satisfying

$$(1.17) \quad \begin{aligned} v_L(\mathbf{x}, \mathbf{y}) &= v_L(\mathbf{x} + \mathbf{z}, \mathbf{y} + \mathbf{z}) = v_L(\mathbf{y}, \mathbf{x}) = v_L(\mathbf{x} + L\mathbf{e}_j, \mathbf{y}), \\ &\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{Z}^d, j \in \{1, \dots, d\}, \\ \sum_{\mathbf{x} \in \Gamma} |v_L(\mathbf{x}, \mathbf{0}) - L^{-d}| &\leq c(d)L^{-d} \end{aligned}$$

with  $c(d) (\in \mathbb{R}_{>0})$  depending only on  $d$ , then the same free energy density as that for (1.15) can be derived in a way parallel to [23], [24], [25]. This is because the difference between (1.15) and (1.16) is measured by the left-hand side of (1.17) and is bounded by  $c(d)L^{-d}$ . A concrete example is that

$$v_L(\mathbf{x}, \mathbf{y}) = L^{-d} + 1_{\mathbf{x} \neq \mathbf{y} \text{ in } (\mathbb{Z}/L\mathbb{Z})^d} \exp \left( -L^{1+d} \sum_{j=1}^d |e^{i\frac{2\pi}{L}(x_j - y_j)} - 1| \right).$$

At present we cannot give an example of interaction for which an essentially different free energy density from that for (1.15) can be derived under the influence of imaginary magnetic field.

**Remark 1.14.** In Subsection 1.1 we noted that there is no EPT in the BCS model with real magnetic field  $\mathbf{H} + \theta \mathbf{S}_z$  ( $\theta \in \mathbb{R}$ ) when the BCS interaction is weak and the temperature is high. As the necessary notations are introduced by now, let us explain more explicitly. Let  $E \in \mathcal{E}(e_{\min}, e_{\max})$ . We can reconstruct the framework [23] to prove the following. There exist  $c(b, d, E) \in (0, 1]$  depending only on  $b, d, E, n(d) \in \mathbb{N}$  depending only on  $d$  such that for any  $\theta \in \mathbb{R}, \beta \in \mathbb{R}_{>0}$ ,

$$(1.18) \quad U \in \left[ -\min \left\{ c(b, d, E)(1 + \beta)^{-n(d)}, \frac{2e_{\min}}{b} \right\}, 0 \right)$$

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

Since  $|U| \leq \frac{2e_{\min}}{b}$ , the corresponding gap equation

$$(1.20) \quad -\frac{2}{|U|} + D_d \int_{\Gamma_{\infty}^*} d\mathbf{k} \text{Tr} \left( \frac{\sinh(\beta \sqrt{E(\mathbf{k})^2 + \Delta^2})}{(\cosh(\beta\theta/2) + \cosh(\beta \sqrt{E(\mathbf{k})^2 + \Delta^2})) \sqrt{E(\mathbf{k})^2 + \Delta^2}} \right) = 0$$

has no solution. Indeed (L.H.S of (1.20))  $< -\frac{2}{|U|} + \frac{b}{e_{\min}} \leq 0$  for any  $\Delta \in \mathbb{R}$ . This is the reason why the right-hand side of (1.19) does not contain the gap function  $\Delta$ .

We want to have the equality (1.19) for  $\beta \in (0, \beta_c)$  where the DQPT takes place. For this purpose we further assume that

$$U \in \left[ -\min \left\{ c(b, d, E) 2^{-n(d)}, \frac{2e_{\min}}{b} \tanh \left( \frac{e_{\min}}{2} \right) \right\}, 0 \right).$$

It follows from Lemma 1.3 that  $\beta_c \leq 1$ . For any  $\beta \in (0, \beta_c]$   $U$  satisfies (1.18), and thus (1.19) holds. Since the right-hand side of (1.19) is analytic with  $(\beta, \theta)$

in  $(0, \beta_c) \times \mathbb{R}$ , there is no EPT driven by  $(\beta, \theta)$  in  $(0, \beta_c) \times \mathbb{R}$ . Though we cannot derive the zero-temperature limit of the free energy density within our framework, at least we can formally extract some hint of existence of critical magnetic fields at zero temperature. Observe that

$$\lim_{\beta \rightarrow \infty} (\text{R.H.S of (1.19)}) = -D_d \int_{\Gamma_\infty^*} d\mathbf{k} \text{Tr} \left( \max \left\{ \frac{|\theta|}{2}, |E(\mathbf{k})| \right\} \right) + D_d \int_{\Gamma_\infty^*} d\mathbf{k} \text{Tr} E(\mathbf{k}),$$

which is not analytic with  $\theta$  in  $\mathbb{R}$  and singular points exist in  $[-2e_{\max}, -2e_{\min}] \cup [2e_{\min}, 2e_{\max}]$ . For example if

$$E(\mathbf{k}) = \begin{pmatrix} e_{\min} & 0 \\ 0 & e_{\max} \end{pmatrix}$$

with any  $e_{\min}, e_{\max} \in \mathbb{R}_{>0}$  satisfying  $e_{\min} \leq e_{\max}$ ,  $d \in \mathbb{N}$  and basis  $(\mathbf{v}_j)_{j=1}^d$  of  $\mathbb{R}^d$ ,

$$\lim_{\beta \rightarrow \infty} (\text{R.H.S of (1.19)}) = -\max \left\{ \frac{|\theta|}{2}, e_{\min} \right\} - \max \left\{ \frac{|\theta|}{2}, e_{\max} \right\} + e_{\min} + e_{\max}.$$

Therefore  $\theta = \pm 2e_{\min}, \pm 2e_{\max}$  are critical points at zero temperature. However, our DQPTs occur at positive temperatures whether the quench from  $\mathbf{H}$  to  $\mathbf{H} + \theta \mathbf{S}_z$  ( $\theta \in \mathbb{R} \setminus \{0\}$ ) crosses these critical points or not.

## 2 Proof of the main results

In this section we will prove Theorem 1.6, Theorem 1.7 and Theorem 1.8. The proof of Theorem 1.6 will be completed in Subsection 2.1. We decompose Theorem 1.7, Theorem 1.8 into several claims. We will prove the claims step by step. Combination of them will complete the proof of Theorem 1.7, Theorem 1.8 in the end of this section.

### 2.1 HOPT and SPI

Here we prove Theorem 1.6, the equivalence between the claim (i) and the claim (ii) of Theorem 1.7 and the equivalence between the claim (i), the claim (ii) and the claim (iii) of Theorem 1.8. To this end, we define the functions  $\tilde{F}_E, \tilde{g}_E : \mathbb{R}_{>0} \times \mathbb{R} \times (-e_{\min}^2, \infty) \rightarrow \mathbb{R}$  for  $E \in \mathcal{E}(e_{\min}, e_{\max})$  by

$$\begin{aligned} \tilde{F}_E(x, t, z) &:= \frac{z}{|U|} - \frac{D_d}{x} \int_{\Gamma_\infty^*} d\mathbf{k} \text{Tr} \log \left( \cos \left( \frac{t}{2} \right) + \cosh(x\sqrt{E(\mathbf{k})^2 + z}) \right), \\ \tilde{g}_E(x, t, z) &:= -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k} \text{Tr} \left( \frac{\sinh(x\sqrt{E(\mathbf{k})^2 + z})}{(\cos(t/2) + \cosh(x\sqrt{E(\mathbf{k})^2 + z}))\sqrt{E(\mathbf{k})^2 + z}} \right). \end{aligned}$$

Observe that

$$(2.1) \quad F_E(\beta, t) = \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) - \frac{D_d}{\beta} \int_{\Gamma_\infty^*} d\mathbf{k} \text{Tr} \log(2e^{-\beta E(\mathbf{k})}), \quad \forall (\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R},$$

$$(2.2) \quad g_E(x, t, z) = \tilde{g}_E(x, t, z^2),$$

$$(2.3) \quad \frac{\partial \tilde{F}_E}{\partial z}(x, t, z) = -\frac{1}{2} \tilde{g}_E(x, t, z),$$

$$(2.4) \quad \frac{\partial \tilde{g}_E}{\partial z}(x, t, z) < 0, \quad \forall (x, t, z) \in \mathbb{R}_{>0} \times \mathbb{R} \times (-e_{min}^2, \infty).$$

The inequality (2.4) is based on the fact that

$$(2.5) \quad x \mapsto \frac{\sinh x}{(\varepsilon + \cosh x)x} : \mathbb{R}_{>0} \rightarrow \mathbb{R}$$

is strictly monotone decreasing for any  $\varepsilon \in [-1, 1]$ . The equality (2.1) suggests that we can study the regularity of the function  $F_E$  by analyzing  $\tilde{F}_E(\beta, t, \Delta(\beta, t)^2)$  instead. It follows from (1.14), (2.1) that

$$(2.6) \quad (\beta, t) \mapsto \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) \text{ is real analytic in } Q_+ \cup Q_- \text{ and } C^1\text{-class in } \mathbb{R}_{>0} \times \mathbb{R}.$$

We can see from this fact and the inequality (2.4) that the statement of the next lemma makes sense.

**Lemma 2.1.** *For any  $n \in \mathbb{N}_{\geq 2}$  ( $= \{2, 3, 4, \dots\}$ ) and  $(\beta, t) \in Q_+$  the following equality holds.*

$$(2.7) \quad \begin{aligned} & \left( \frac{\partial}{\partial \beta} \right)^n \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) \\ &= \frac{\partial^n \tilde{F}_E}{\partial x^n}(\beta, t, \Delta(\beta, t)^2) \\ &+ \frac{1}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta, t, \Delta(\beta, t)^2)} \sum_{j=0}^{n-2} \left( \frac{\partial}{\partial x} \right)^j \left( \frac{\partial \tilde{g}_E}{\partial x}(x, t, z) \frac{\partial^{n-1-j} \tilde{g}_E}{\partial x^{n-1-j}}(x, t, z) \right) \Big|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}} \\ &+ \sum_{\rho, \eta \in \mathbb{N}_{\geq 1}} 1_{\rho \leq \eta} 1_{\rho + \eta \leq n-1} P_{\rho, \eta} \left( \left( \frac{\partial \tilde{g}_E}{\partial z}(x, t, z) \right)^{-1}, \left( \frac{\partial^{a+b} \tilde{g}_E}{\partial x^a \partial z^b}(x, t, z) \right)_{\substack{a, b \in \mathbb{N} \cup \{0\} \\ 1 \leq a+b \leq n-1}} \right) \\ & \cdot \frac{\partial^\rho \tilde{g}_E}{\partial x^\rho}(x, t, z) \frac{\partial^\eta \tilde{g}_E}{\partial x^\eta}(x, t, z) \Big|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}}. \end{aligned}$$

Here  $P_{\rho, \eta}$  is a polynomial with real coefficient for any  $\rho, \eta \in \mathbb{N}_{\geq 1}$  satisfying  $\rho \leq \eta$ ,  $\rho + \eta \leq n-1$ . For  $C_{a,b} \in \mathbb{C}$  ( $a, b \in \mathbb{N} \cup \{0\}$ ,  $1 \leq a+b \leq n-1$ )

$$(C_{a,b})_{\substack{a, b \in \mathbb{N} \cup \{0\} \\ 1 \leq a+b \leq n-1}} := (C_{0,1}, C_{0,2}, \dots, C_{0,n-1}, C_{1,0}, C_{1,1}, \dots, C_{1,n-2}, \dots, C_{n-1,0}).$$

*Proof.* Take any  $(\beta, t) \in Q_+$ . By (2.3)

$$\frac{\partial}{\partial \beta} \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) = \frac{\partial \tilde{F}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2) - \Delta(\beta, t) \frac{\partial \Delta}{\partial \beta}(\beta, t) \tilde{g}_E(\beta, t, \Delta(\beta, t)^2).$$

Here we remark that by the implicit function theorem for real analytic functions (see e.g. [26])  $\Delta \in C^\omega(Q_+ \cup Q_-)$ . By (2.2)  $\tilde{g}_E(\beta, t, \Delta(\beta, t)^2) = 0$ . Thus,

$$\frac{\partial}{\partial \beta} \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) = \frac{\partial \tilde{F}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2).$$

Moreover, by (2.3)

$$\begin{aligned} (2.8) \quad & \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) \\ &= \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta, t, \Delta(\beta, t)^2) + 2\Delta(\beta, t) \frac{\partial \Delta}{\partial \beta}(\beta, t) \frac{\partial^2 \tilde{F}_E}{\partial x \partial z}(\beta, t, \Delta(\beta, t)^2) \\ &= \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta, t, \Delta(\beta, t)^2) - \Delta(\beta, t) \frac{\partial \Delta}{\partial \beta}(\beta, t) \frac{\partial \tilde{g}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2). \end{aligned}$$

We can derive from (2.2), (2.4) that

$$(2.9) \quad \Delta(\beta, t) \frac{\partial \Delta}{\partial \beta}(\beta, t) = -\frac{\frac{\partial \tilde{g}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2)}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta, t, \Delta(\beta, t)^2)}.$$

By substituting (2.9) into (2.8) we obtain that

$$\left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) = \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta, t, \Delta(\beta, t)^2) + \frac{\left( \frac{\partial \tilde{g}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2) \right)^2}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta, t, \Delta(\beta, t)^2)},$$

which is (2.7) for  $n = 2$ .

Let us assume that (2.7) holds for some  $n \in \mathbb{N}_{\geq 2}$ . By differentiating both sides with  $\beta$  and using (2.3), (2.9) we have that

$$\begin{aligned} (2.10) \quad & \left( \frac{\partial}{\partial \beta} \right)^{n+1} \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) \\ &= \frac{\partial^{n+1} \tilde{F}_E}{\partial x^{n+1}}(\beta, t, \Delta(\beta, t)^2) + \frac{\frac{\partial \tilde{g}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2) \frac{\partial^n \tilde{g}_E}{\partial x^n}(\beta, t, \Delta(\beta, t)^2)}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta, t, \Delta(\beta, t)^2)} \\ &+ \frac{1}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta, t, \Delta(\beta, t)^2)} \sum_{j=0}^{n-2} \left( \frac{\partial}{\partial x} \right)^{j+1} \left( \frac{\partial \tilde{g}_E}{\partial x}(x, t, z) \frac{\partial^{n-1-j} \tilde{g}_E}{\partial x^{n-1-j}}(x, t, z) \right) \Big|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}} \\ &+ \frac{\partial}{\partial x} \left( \frac{1}{2 \frac{\partial \tilde{g}_E}{\partial z}(x, t, z)} \right) \Big|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}} \\ &\cdot \sum_{j=0}^{n-2} \left( \frac{\partial}{\partial x} \right)^j \left( \frac{\partial \tilde{g}_E}{\partial x}(x, t, z) \frac{\partial^{n-1-j} \tilde{g}_E}{\partial x^{n-1-j}}(x, t, z) \right) \Big|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}} \\ &- \frac{\frac{\partial \tilde{g}_E}{\partial x}(\beta, t, \Delta(\beta, t)^2)}{\frac{\partial \tilde{g}_E}{\partial z}(\beta, t, \Delta(\beta, t)^2)} \\ &\cdot \frac{\partial}{\partial z} \left( \frac{1}{2 \frac{\partial \tilde{g}_E}{\partial z}(x, t, z)} \sum_{j=0}^{n-2} \left( \frac{\partial}{\partial x} \right)^j \left( \frac{\partial \tilde{g}_E}{\partial x}(x, t, z) \frac{\partial^{n-1-j} \tilde{g}_E}{\partial x^{n-1-j}}(x, t, z) \right) \right) \Big|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}} \end{aligned}$$

$$\begin{aligned}
& + \sum_{\rho, \eta \in \mathbb{N}_{\geq 1}} 1_{\rho \leq \eta} 1_{\rho + \eta \leq n-1} \left( \frac{\partial}{\partial x} - \frac{\frac{\partial \tilde{g}_E}{\partial x}(x, t, z)}{\frac{\partial \tilde{g}_E}{\partial z}(x, t, z)} \frac{\partial}{\partial z} \right) \\
& \cdot \left( P_{\rho, \eta} \left( \left( \frac{\partial \tilde{g}_E}{\partial z}(x, t, z) \right)^{-1}, \left( \frac{\partial^{a+b} \tilde{g}_E}{\partial x^a \partial z^b}(x, t, z) \right) \right. \right. \\
& \left. \left. \left. \left. \frac{\partial^\rho \tilde{g}_E}{\partial x^\rho}(x, t, z) \frac{\partial^\eta \tilde{g}_E}{\partial x^\eta}(x, t, z) \right) \right|_{\substack{x=\beta, \\ z=\Delta(\beta, t)^2}} \right) .
\end{aligned}$$

For any smooth function  $f(x)$

$$(2.11) \quad \sum_{j=0}^{n-2} \left( \frac{d}{dx} \right)^j \left( \frac{df}{dx}(x) \frac{d^{n-1-j} f}{dx^{n-1-j}}(x) \right) = \sum_{k=1}^{n-1} \sum_{j=k}^{n-1} \binom{j-1}{k-1} \frac{d^k f}{dx^k}(x) \frac{d^{n-k} f}{dx^{n-k}}(x),$$

$$(2.12) \quad \sum_{j=0}^{n-2} \left( \frac{d}{dx} \right)^{j+1} \left( \frac{df}{dx}(x) \frac{d^{n-1-j} f}{dx^{n-1-j}}(x) \right) = \sum_{j=1}^{n-1} \left( \frac{d}{dx} \right)^j \left( \frac{df}{dx}(x) \frac{d^{n-j} f}{dx^{n-j}}(x) \right).$$

By using (2.11), (2.12) for  $f(x) = \tilde{g}_E(x, t, z)$  we can see that the 1st, 2nd, 3rd term of the right side of (2.10) can be organized into the 1st, 2nd term of the right side of (2.7) for  $n+1$  and the 4th, 5th, 6th term of (2.10) can be summarized into the last term of the right side of (2.7) for  $n+1$ . Thus, (2.7) holds for  $n+1$ . The induction with  $n$  concludes the proof.  $\square$

To understand the following lemmas, let us recall that  $\tau \in C^\omega((0, \beta_c))$ , which is claimed in [25, Lemma 2.2 (i)].

**Lemma 2.2.** (i)

$$\frac{\partial \tilde{g}_E}{\partial x}(\beta, \tau(\beta), 0) = -\frac{\partial \tilde{g}_E}{\partial t}(\beta, \tau(\beta), 0) \frac{d\tau}{d\beta}(\beta), \quad \forall \beta \in (0, \beta_c).$$

(ii) Assume that  $\beta_0 \in (0, \beta_c)$ ,  $n \in \mathbb{N}_{\geq 2}$  and

$$\frac{d^m \tau}{d\beta^m}(\beta_0) = 0, \quad \forall m \in \{1, 2, \dots, n-1\}.$$

Then

$$\begin{aligned}
& \frac{\partial^m \tilde{g}_E}{\partial x^m}(\beta_0, \tau(\beta_0), 0) = 0, \quad \forall m \in \{0, 1, \dots, n-1\}, \\
& \frac{\partial^n \tilde{g}_E}{\partial x^n}(\beta_0, \tau(\beta_0), 0) = -\frac{\partial \tilde{g}_E}{\partial t}(\beta_0, \tau(\beta_0), 0) \frac{d^n \tau}{d\beta^n}(\beta_0).
\end{aligned}$$

*Proof.* (i): The claim follows from the equality

$$(2.13) \quad \tilde{g}_E(\beta, \tau(\beta), 0) = 0, \quad \forall \beta \in (0, \beta_c).$$

(ii): We can derive from (2.13) that

$$\left( \frac{\partial}{\partial x} + \frac{d\tau}{dx}(x) \frac{\partial}{\partial t} \right)^l \tilde{g}_E(x, t, 0) \Big|_{\substack{x=\beta, \\ t=\tau(\beta)}} = 0, \quad \forall l \in \mathbb{N} \cup \{0\}, \quad \beta \in (0, \beta_c).$$

The result follows from this equality and the assumption.  $\square$

**Lemma 2.3.** Assume that  $\beta_0$  ( $\in (0, \beta_c)$ ) is a SPI of  $\tau(\cdot)$ . Then there exist  $n \in 2\mathbb{N}+1$  ( $= \{3, 5, 7, \dots\}$ ) and  $\varepsilon \in \mathbb{R}_{>0}$  such that  $(\beta_0 - \varepsilon, \beta_0 + \varepsilon) \subset (0, \beta_c)$  and

$$\begin{aligned} \frac{d^m \tau}{d\beta^m}(\beta_0) &= 0, \quad \forall m \in \{1, 2, \dots, n-1\}, \\ \frac{d^n \tau}{d\beta^n}(\beta_0) &\neq 0, \\ \frac{d\tau}{d\beta}(\beta) &\neq 0, \quad \forall \beta \in (\beta_0 - \varepsilon, \beta_0 + \varepsilon) \setminus \{\beta_0\}. \end{aligned}$$

Moreover,

$$\begin{aligned} (2.14) \quad \frac{\partial^m \tilde{g}_E}{\partial x^m}(\beta_0, \tau(\beta_0), 0) &= 0, \quad \forall m \in \{0, 1, \dots, n-1\}, \\ \frac{\partial^n \tilde{g}_E}{\partial x^n}(\beta_0, \tau(\beta_0), 0) &\neq 0. \end{aligned}$$

*Proof.* The claims on  $\tau(\cdot)$  are general properties of a real analytic function having a SPI. However, we provide the proof for clarity. By the assumption and the definition of SPI there exists  $\varepsilon \in \mathbb{R}_{>0}$  such that  $(\beta_0 - \varepsilon, \beta_0 + \varepsilon) \subset (0, \beta_c)$ ,  $\frac{d\tau}{d\beta}(\beta_0) = 0$  and

$$(2.15) \quad \frac{d\tau}{d\beta}(\beta) > 0, \quad \forall \beta \in (\beta_0 - \varepsilon, \beta_0 + \varepsilon) \setminus \{\beta_0\} \quad \text{or} \quad \frac{d\tau}{d\beta}(\beta) < 0, \quad \forall \beta \in (\beta_0 - \varepsilon, \beta_0 + \varepsilon) \setminus \{\beta_0\}.$$

Since  $\tau \in C^\omega((0, \beta_c))$ , there exist  $\varepsilon' \in (0, \varepsilon]$ ,  $n \in \mathbb{N}_{\geq 2}$  such that  $\frac{d^m \tau}{d\beta^m}(\beta_0) = 0$ ,  $\forall m \in \{1, 2, \dots, n-1\}$ ,  $\frac{d^n \tau}{d\beta^n}(\beta_0) \neq 0$  and

$$\frac{d\tau}{d\beta}(\beta) = \sum_{m=n}^{\infty} \frac{1}{(m-1)!} \frac{d^m \tau}{d\beta^m}(\beta_0) (\beta - \beta_0)^{m-1}, \quad \forall \beta \in (\beta_0 - \varepsilon', \beta_0 + \varepsilon').$$

We can deduce from the property (2.15) and the above expansion that  $n$  must be odd. At this point the claims on  $\tau(\cdot)$  have been proved. The claims on  $\tilde{g}_E$  follow from the above properties of  $\tau(\cdot)$  and Lemma 2.2 (ii) plus the fact  $\frac{\partial \tilde{g}_E}{\partial t}(\beta_0, \tau(\beta_0), 0) > 0$  based on  $\tau(\beta_0) \in (\pi, 2\pi)$ .  $\square$

We can prove Theorem 1.6 by applying Lemma 2.1 and Lemma 2.3.

*Proof of Theorem 1.6.* (i): Assume that  $(\text{SPI})_\xi(\beta_0)$  holds. We can see from (1.13) and the general behavior of  $\tau(\cdot)$  proved in [25, Lemma 2.2] that  $(\beta_0, \tau(\beta_0)) \in Q_{\rho, n}$ . By Lemma 2.3 there exists  $n_0 \in 2\mathbb{N}+1$  such that (2.14) holds for  $n = n_0$ . We remark that

$$(2.16) \quad \left( \frac{\partial}{\partial \beta} \right)^l \tilde{F}_E(\beta, t, \Delta(\beta, t)^2) = \frac{\partial^l \tilde{F}_E}{\partial x^l}(\beta, t, 0), \quad \forall (\beta, t) \in Q_-, \quad l \in \mathbb{N} \cup \{0\}.$$

Bearing (2.11) in mind, we observe that for any  $n \in \{2, 3, \dots, 2n_0 - 1\}$  each of the 2nd, 3rd terms of the right-hand side of (2.7) contains  $\frac{\partial^m \tilde{g}_E}{\partial x^m}(\beta, t, \Delta(\beta, t)^2)$  for some  $m \in \{1, 2, \dots, n_0 - 1\}$ . For  $n = 2n_0$  the 2nd term contains  $(\frac{\partial^{n_0} \tilde{g}_E}{\partial x^{n_0}}(\beta, t, \Delta(\beta, t)^2))^2$  and each of the 3rd terms contains  $\frac{\partial^m \tilde{g}_E}{\partial x^m}(\beta, t, \Delta(\beta, t)^2)$  for some  $m \in \{1, 2, \dots, n_0 - 1\}$ .

$1\}$ . This observation and the properties (2.4), (2.14), (2.16) imply that for any  $n \in \{2, 3, \dots, 2n_0 - 1\}$

$$\begin{aligned}
& \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_+}} \left( \frac{\partial}{\partial \beta} \right)^n \tilde{F}_E(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2) \\
&= \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_+}} \frac{\partial^n \tilde{F}_E}{\partial x^n}(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2) \\
&= \frac{\partial^n \tilde{F}_E}{\partial x^n}(\beta_0, \tau(\beta_0), 0) \\
&= \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_-}} \left( \frac{\partial}{\partial \beta} \right)^n \tilde{F}_E(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2), \\
& \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_+}} \left( \frac{\partial}{\partial \beta} \right)^{2n_0} \tilde{F}_E(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2) \\
&= \frac{\partial^{2n_0} \tilde{F}_E}{\partial x^{2n_0}}(\beta_0, \tau(\beta_0), 0) + \frac{\sum_{j=n_0}^{2n_0-1} \binom{j-1}{n_0-1}}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta_0, \tau(\beta_0), 0)} \left( \frac{\partial^{n_0} \tilde{g}_E}{\partial x^{n_0}}(\beta_0, \tau(\beta_0), 0) \right)^2 \\
&< \frac{\partial^{2n_0} \tilde{F}_E}{\partial x^{2n_0}}(\beta_0, \tau(\beta_0), 0) \\
&= \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_-}} \left( \frac{\partial}{\partial \beta} \right)^{2n_0} \tilde{F}_E(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2).
\end{aligned}$$

Combined with (2.1), the above argument concludes that  $(\text{PT})_{2n_0, (\rho, \eta)}(\beta_0, \tau(\beta_0))$  holds.

Assume that  $(\text{SPI})_\xi(\beta_0)$  does not hold and  $(\beta_0, \tau(\beta_0)) \in Q_{\rho, \eta}$ . It follows from (1.12), (1.13) that  $\frac{d\tau}{d\beta}(\beta_0) \geq 0$  if  $\xi = r$ ,  $\frac{d\tau}{d\beta}(\beta_0) \leq 0$  if  $\xi = f$ . Consider the case that  $\xi = r$  and  $\frac{d\tau}{d\beta}(\beta_0) = 0$ . Since  $\tau(\cdot)$  is real analytic and not constant, there exists  $\varepsilon \in \mathbb{R}_{>0}$  such that  $\frac{d\tau}{d\beta}(\beta) \neq 0$ ,  $\forall \beta \in (\beta_0 - \varepsilon, \beta_0 + \varepsilon) \setminus \{\beta_0\}$ . If  $\frac{d\tau}{d\beta}(\beta) < 0$ ,  $\forall \beta \in (\beta_0 - \varepsilon, \beta_0)$  or  $\frac{d\tau}{d\beta}(\beta) > 0$ ,  $\forall \beta \in (\beta_0, \beta_0 + \varepsilon)$ , it contradicts that  $(\beta_0, \tau(\beta_0)) \in Q_{+, -}$ . Thus  $\frac{d\tau}{d\beta}(\beta) > 0$ ,  $\forall \beta \in (\beta_0 - \varepsilon, \beta_0 + \varepsilon) \setminus \{\beta_0\}$ , which means that  $\beta_0$  is a rising SPI, a contradiction. Therefore  $\frac{d\tau}{d\beta}(\beta_0) > 0$  if  $\xi = r$ . Similarly we can prove that  $\frac{d\tau}{d\beta}(\beta_0) < 0$  if  $\xi = f$ .

We can derive from this, (2.7) for  $n = 2$ , Lemma 2.2 (i) and (2.16) that

$$\begin{aligned}
& \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_+}} \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2) \\
&= \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta_0, \tau(\beta_0), 0) + \frac{(\frac{\partial \tilde{g}_E}{\partial t}(\beta_0, \tau(\beta_0), 0) \frac{d\tau}{d\beta}(\beta_0))^2}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta_0, \tau(\beta_0), 0)} \\
&< \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta_0, \tau(\beta_0), 0) \\
&= \lim_{\substack{\beta \rightarrow \beta_0 \\ (\beta, \tau(\beta_0)) \in Q_-}} \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, \tau(\beta_0), \Delta(\beta, \tau(\beta_0))^2).
\end{aligned}$$

Here we also used (2.4) and that  $\frac{\partial \tilde{g}_E}{\partial t}(\beta_0, \tau(\beta_0), 0) > 0$ . This together with (2.1), (2.6) imply that  $(\text{PT})_{2,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  holds, and thus  $(\text{PT})_{n,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  does not hold for any  $n \in 4\mathbb{N} + 2$ . If  $(\beta_0, \tau(\beta_0)) \notin Q_{\rho,\eta}$ ,  $(\text{PT})_{n,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  does not hold for any  $n \in 4\mathbb{N} + 2$  by definition. The claim (i) is proved.

(ii): Assume that  $(\text{SPI})_\xi$  does not hold. Take any  $(\beta_1, t_1) \in Q_{\rho,\eta}$ . First let us assume that  $\beta_1 \in (0, \beta_c)$ . It follows from (1.12), (1.13) that  $(\beta_1, \tau(\beta_1)) \in Q_{\rho,\eta}$ . The same argument as in the 2nd half of the proof of (i) leads to that

$$\begin{aligned} & \lim_{\substack{\beta \rightarrow \beta_1 \\ (\beta, \tau(\beta_1)) \in Q_+}} \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, \tau(\beta_1), \Delta(\beta, \tau(\beta_1))^2) \\ & < \lim_{\substack{\beta \rightarrow \beta_1 \\ (\beta, \tau(\beta_1)) \in Q_-}} \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, \tau(\beta_1), \Delta(\beta, \tau(\beta_1))^2). \end{aligned}$$

This property, (2.1) and (2.6) ensure that  $(\text{PT})_{2,(\rho,\eta)}(\beta_1, \tau(\beta_1))$  holds. Then by Lemma 1.4  $(\text{PT})_{2,(\rho,\eta)}(\beta_1, t_1)$  holds.

Next let us assume that  $\beta_1 = \beta_c$ . In this case

$$\tilde{g}_E(x, t_1, 0) = -\frac{2}{|U|} + D_d \int_{\Gamma_\infty^*} d\mathbf{k} \text{Tr} \left( \frac{1}{\tanh(\frac{x}{2}|E(\mathbf{k})|)|E(\mathbf{k})|} \right), \quad \forall x \in \mathbb{R}_{>0},$$

and thus  $\frac{\partial \tilde{g}_E}{\partial x}(x, t_1, 0) < 0, \forall x \in \mathbb{R}_{>0}$ . Using this inequality, (2.4), (2.7) for  $n = 2$  and (2.16), we deduce that

$$\begin{aligned} & \lim_{\substack{\beta \rightarrow \beta_1 \\ (\beta, t_1) \in Q_+}} \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, t_1, \Delta(\beta, t_1)^2) = \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta_1, t_1, 0) + \frac{(\frac{\partial \tilde{g}_E}{\partial x}(\beta_1, t_1, 0))^2}{2 \frac{\partial \tilde{g}_E}{\partial z}(\beta_1, t_1, 0)} \\ & < \frac{\partial^2 \tilde{F}_E}{\partial x^2}(\beta_1, t_1, 0) \\ & = \lim_{\substack{\beta \rightarrow \beta_1 \\ (\beta, t_1) \in Q_-}} \left( \frac{\partial}{\partial \beta} \right)^2 \tilde{F}_E(\beta, t_1, \Delta(\beta, t_1)^2), \end{aligned}$$

which together with (2.1), (2.6) imply that  $(\text{PT})_{2,(\rho,\eta)}(\beta_1, t_1)$  holds. Thus we have proved that if  $(\text{SPI})_\xi$  does not hold,  $(\text{PT})_{2,(\rho,\eta)}(\beta, t)$  holds for any  $(\beta, t) \in Q_{\rho,\eta}$ .

If  $(\text{SPI})_\xi$  holds, by the claim (i) there exist  $\beta_2 \in (0, \beta_c)$ ,  $n \in 4\mathbb{N} + 2$  such that  $(\text{PT})_{n,(\rho,\eta)}(\beta_2, \tau(\beta_2))$  holds. This means that  $(\beta_2, \tau(\beta_2)) \in Q_{\rho,\eta}$  and  $(\text{PT})_{2,(\rho,\eta)}(\beta_2, \tau(\beta_2))$  does not hold. We have proved the claim (ii).

(iii): Assume that  $(\beta_3, t_3) \in Q_{\rho,\eta}$  and  $(\text{PT})_{2,(\rho,\eta)}(\beta_3, t_3)$  does not hold. If  $\beta_3 = \beta_c$ , by the 2nd half of the proof of (ii)  $(\text{PT})_{2,(\rho,\eta)}(\beta_3, t_3)$  holds, which is a contradiction. Thus  $\beta_3 \in (0, \beta_c)$ . If  $(\text{SPI})_\xi(\beta_3)$  does not hold, by the 1st half of the proof of (ii)  $(\text{PT})_{2,(\rho,\eta)}(\beta_3, t_3)$  holds, contradicting the assumption. Thus  $(\text{SPI})_\xi(\beta_3)$  must hold. Then by the 1st half of the proof of (i) there exists  $n \in 4\mathbb{N} + 2$  such that  $(\text{PT})_{n,(\rho,\eta)}(\beta_3, \tau(\beta_3))$  holds. Moreover, by Lemma 1.4  $(\text{PT})_{n,(\rho,\eta)}(\beta_3, t_3)$  holds. The converse is obvious from the definition.  $\square$

As a corollary of Theorem 1.6, we can prove the following.

**Corollary 2.4.** (1) The statements (i), (ii) of Theorem 1.7 are equivalent to each other.

(2) The statements (i), (ii), (iii) of Theorem 1.8 are equivalent to each other.

*Proof.* (1): If  $(\text{PT})_{n,(\rho,\eta)}$  holds with  $n \in 4\mathbb{N} + 2$ , by Lemma 1.4 there exists  $\beta_0 \in (0, \beta_c]$  such that  $(\text{PT})_{n,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  holds if  $\beta_0 < \beta_c$ ,  $(\text{PT})_{n,(\rho,\eta)}(\beta_0, 2\pi)$  holds if  $\beta_0 = \beta_c$ . If  $\beta_0 = \beta_c$ , it follows from the proof of Theorem 1.6 (ii) above that  $(\text{PT})_{2,(\rho,\eta)}(\beta_0, 2\pi)$  holds, which is a contradiction. Thus  $\beta_0 < \beta_c$  and  $(\text{PT})_{n,(\rho,\eta)}(\beta_0, \tau(\beta_0))$  holds. We can deduce the equivalence between (i) and (ii) of Theorem 1.7 from the above argument and Theorem 1.6 (i).

(2): Theorem 1.6 (ii) implies the equivalence between the statements (ii), (iii). We can deduce from the definition of  $(\text{PT})_{n,(\rho,\eta)}$  that the statement (ii) implies the statement (i). It suffices to show that the statement (i) implies the statement (iii). Suppose that for any  $U_0 \in (0, \frac{2e_{\min}}{b})$  there exist  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{\min}, e_{\max})$ ,  $\xi \in \{r, f\}$  such that  $(\text{SPI})_\xi$  holds. By definition there exists  $\beta_0 \in (0, \beta_c)$  such that  $(\text{SPI})_\xi(\beta_0)$  holds. Set  $(\rho, \eta) := (+, -)$  if  $\xi = r$ ,  $(-, +)$  if  $\xi = f$ . By Theorem 1.6 (i) there exists  $n \in \mathbb{N}_{\geq 3}$  such that  $(\text{PT})_{n,(\rho,\eta)}$  holds. This means that (i) implies (iii). Thus the claim holds true.  $\square$

The following corollary will be used in Subsection 2.4 and Subsection 2.5 to prove key propositions on which Theorem 1.7, Theorem 1.8 are based.

**Corollary 2.5.** *Under the same assumption of Theorem 1.6 the following statement holds.  $(\text{SPI})_\xi$  holds if and only if there exists  $n \in 4\mathbb{N} + 2$  such that  $(\text{PT})_{n,(\rho,\eta)}$  holds.*

*Proof.* By Theorem 1.6 (i), if  $(\text{SPI})_\xi$  holds, there exists  $n \in 4\mathbb{N} + 2$  such that  $(\text{PT})_{n,(\rho,\eta)}$  holds. It follows from the 2nd half of the proof of Theorem 1.6 (ii) and (1.12), (1.13) that  $(\text{PT})_{2,(+,-)}(\beta_c, t_1)$  holds for any  $t_1 \in \mathbb{R}$  satisfying  $(\beta_c, t_1) \in Q_{+,-}$  and  $(\beta_c, t) \notin Q_{-,+}$  for any  $t \in \mathbb{R}$ . This ensures that if  $(\text{PT})_{n,(\rho,\eta)}(\beta, t)$  holds for some  $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$ ,  $n \in 4\mathbb{N} + 2$ , then  $\beta \in (0, \beta_c)$ . We can deduce from this property, Lemma 1.4, Theorem 1.6 (i) that if there exists  $n \in 4\mathbb{N} + 2$  such that  $(\text{PT})_{n,(\rho,\eta)}$  holds,  $(\text{SPI})_\xi$  holds.  $\square$

## 2.2 General lemmas

Here we prepare several lemmas in order to prove Theorem 1.7, Theorem 1.8 in the following subsections. For  $E \in \mathcal{E}(e_{\min}, e_{\max})$  we define the function  $F_\infty : \mathbb{R} \times (-1, 0) \rightarrow \mathbb{R}$  by

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

In fact this function was defined in [25, (2.38)]. We keep using the same notation for consistency with the previous paper. First of all let us state a basic lemma which follows from Lemma 1.3 and is the same as [25, Lemma 2.1]. Presenting the whole statement here must be convenient for the readers to apply in the subsequent construction.

**Lemma 2.6.** *Assume that  $|U| < \frac{2e_{\min}}{b}$ ,  $y \in (-1, 0)$ ,  $\beta \in \mathbb{R}_{>0}$ ,  $E \in \mathcal{E}(e_{\min}, e_{\max})$  and  $\frac{2}{|U|} = F_\infty(\beta, y)$ . Then  $\beta \in (0, \beta_c)$  and  $y = \cos(\frac{\tau(\beta)}{2})$ .*

The next lemma gives a sufficient condition in terms of  $F_\infty$  for  $\tau(\cdot)$  not to have any SPI.

**Lemma 2.7.** *Let  $S \subset \mathcal{E}(e_{min}, e_{max})$ ,  $S \neq \emptyset$ . Assume that there exists  $y_0 \in (-1, 0)$  such that for any  $y \in (-1, y_0]$  and  $E \in S$  there uniquely exists  $x_0 \in \mathbb{R}_{>0}$  such that  $\frac{\partial F_\infty}{\partial x}(x_0, y) = 0$ . Then there exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$  and  $E \in S$   $\tau(\cdot)$  has no SPI in  $(0, \beta_c)$ .*

*Proof.* The first half of the proof is close to the initial part of the proof of [25, Proposition 2.8]. Take any  $E \in \mathcal{E}(e_{min}, e_{max})$ . It follows from Lemma 1.3 that for  $U \in (-\frac{2e_{min}}{b}, 0)$

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

By the monotone decreasing property of the function (2.5) and the above inequality

$$\frac{2}{|U|} \leq \frac{b \sinh(\beta e_{min})}{e_{min}(\cos(\tau(\beta)/2) + \cosh(\beta e_{min}))} \leq \frac{b \sinh(2 \tanh^{-1}(1))}{e_{min}(\cos(\tau(\beta)/2) + 1)},$$

and thus

$$\cos \left( \frac{\tau(\beta)}{2} \right) + 1 \leq \frac{b \sinh(2 \tanh^{-1}(1))}{2e_{min}} |U|, \quad \forall \beta \in (0, \beta_c).$$

This implies that there exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$

$$(2.17) \quad \cos \left( \frac{\tau(\beta)}{2} \right) \in (-1, y_0], \quad \forall \beta \in (0, \beta_c).$$

Let us fix  $U \in [-U_0, 0)$  and  $E \in S$ . Suppose that  $\beta_0$  ( $\in (0, \beta_c)$ ) is a SPI of  $\tau(\cdot)$ . Let  $\beta_1 \in (0, \beta_c)$  be a global minimum point of  $\tau(\cdot)$ . Remark that by the behavior of  $\tau(\cdot)$  summarized in [25, Lemma 2.2] a global minimum point exists. By the definition of SPI  $\beta_1 \neq \beta_0$ . Let us assume that  $\beta_1 < \beta_0$ . We can deduce from [25, Lemma 2.2] that there exists  $\beta_2 \in (0, \beta_1]$  such that  $\tau(\beta_2) = \tau(\beta_0)$ . It follows that

$$\frac{2}{|U|} = F_\infty \left( \beta_2, \cos \left( \frac{\tau(\beta_2)}{2} \right) \right) = F_\infty \left( \beta_2, \cos \left( \frac{\tau(\beta_0)}{2} \right) \right) = F_\infty \left( \beta_0, \cos \left( \frac{\tau(\beta_0)}{2} \right) \right).$$

By the mean value theorem there exists  $\beta_3 \in (\beta_2, \beta_0)$  such that

$$(2.18) \quad \frac{\partial F_\infty}{\partial x} \left( \beta_3, \cos \left( \frac{\tau(\beta_0)}{2} \right) \right) = 0.$$

On the other hand, since  $\beta_0$  is a SPI,

$$(2.19) \quad \begin{aligned} 0 &= \frac{\partial F_\infty}{\partial x} \left( \beta_0, \cos \left( \frac{\tau(\beta_0)}{2} \right) \right) - \frac{1}{2} \frac{d\tau}{d\beta}(\beta_0) \sin \left( \frac{\tau(\beta_0)}{2} \right) \frac{\partial F_\infty}{\partial y} \left( \beta_0, \cos \left( \frac{\tau(\beta_0)}{2} \right) \right) \\ &= \frac{\partial F_\infty}{\partial x} \left( \beta_0, \cos \left( \frac{\tau(\beta_0)}{2} \right) \right). \end{aligned}$$

By (2.17)  $\cos(\frac{\tau(\beta_0)}{2}) \in (-1, y_0]$ , which together with (2.18), (2.19) contradict the assumption. Similarly we can derive a contradiction by assuming that  $\beta_1 > \beta_0$ . Therefore  $\tau(\cdot)$  cannot have any SPI in  $(0, \beta_c)$ .  $\square$

The next lemma gives sufficient conditions in terms of  $F_\infty$  for  $\tau(\cdot)$  to have a SPI.

**Lemma 2.8.** *Let  $U_0 \in (0, \frac{2e_{\min}}{b})$ ,  $y_0 \in (-1, 0)$ .*

- (i) *Assume that  $x_0$  is a rising SPI of the function  $x \mapsto F_\infty(x, y_0) : \mathbb{R}_{>0} \rightarrow \mathbb{R}$  and  $F_\infty(x_0, y_0) \geq \frac{2}{U_0}$ . Then there exists  $U \in [-U_0, 0)$  such that  $\tau(\cdot)$  has a falling SPI in  $(0, \beta_c)$ .*
- (ii) *Assume that  $x_0$  is a falling SPI of the function  $x \mapsto F_\infty(x, y_0) : \mathbb{R}_{>0} \rightarrow \mathbb{R}$  and  $F_\infty(x_0, y_0) \geq \frac{2}{U_0}$ . Then there exists  $U \in [-U_0, 0)$  such that  $\tau(\cdot)$  has a rising SPI in  $(0, \beta_c)$ .*

*Proof.* We only give a proof to the claim (i). The claim (ii) can be proved similarly. By the assumption there exist  $\varepsilon \in \mathbb{R}_{>0}$ ,  $U \in [-U_0, 0)$  such that

$$(2.20) \quad \begin{aligned} (x_0 - \varepsilon, x_0 + \varepsilon) &\subset \mathbb{R}_{>0}, \\ \frac{\partial F_\infty}{\partial x}(x_0, y_0) &= 0, \\ \frac{\partial F_\infty}{\partial x}(x, y_0) &> 0, \quad \forall x \in (x_0 - \varepsilon, x_0 + \varepsilon) \setminus \{x_0\}, \\ -\frac{2}{|U|} + F_\infty(x_0, y_0) &= 0. \end{aligned}$$

Here we use Lemma 2.6 to ensure that  $x_0 \in (0, \beta_c)$  and  $y_0 = \cos(\frac{\tau(x_0)}{2})$ . We can derive from the equality  $F_\infty(x, \cos(\frac{\tau(x)}{2})) = \frac{2}{|U|}$  ( $x \in (0, \beta_c)$ ) that

$$0 = \frac{\partial F_\infty}{\partial x}(x_0, y_0) - \frac{1}{2} \sin\left(\frac{\tau(x_0)}{2}\right) \frac{d\tau}{d\beta}(x_0) \frac{\partial F_\infty}{\partial y}(x_0, y_0).$$

It follows from  $\frac{\partial F_\infty}{\partial x}(x_0, y_0) = 0$ ,  $\sin(\frac{\tau(x_0)}{2}) > 0$  and  $\frac{\partial F_\infty}{\partial y}(x_0, y_0) < 0$  that

$$(2.21) \quad \frac{d\tau}{d\beta}(x_0) = 0.$$

By the analytic implicit function theorem (see e.g. [26]) there exist  $\varepsilon_1 \in (0, \varepsilon]$  and a real analytic function  $Y : (x_0 - \varepsilon_1, x_0 + \varepsilon_1) \rightarrow (-1, 0)$  such that

$$\begin{aligned} -\frac{2}{|U|} + F_\infty(x, Y(x)) &= 0, \quad \forall x \in (x_0 - \varepsilon_1, x_0 + \varepsilon_1), \\ Y(x_0) &= y_0. \end{aligned}$$

Let us show that there exists  $\varepsilon_2 \in (0, \varepsilon_1]$  such that

$$(2.22) \quad \begin{aligned} Y(x) &< y_0, \quad \forall x \in (x_0 - \varepsilon_2, x_0), \\ Y(x) &> y_0, \quad \forall x \in (x_0, x_0 + \varepsilon_2). \end{aligned}$$

Suppose that for any  $\varepsilon_3 \in (0, \varepsilon_1]$  there exists  $x_1 \in (x_0 - \varepsilon_3, x_0)$  such that  $Y(x_1) \geq y_0$ . By (2.20) and the fact  $y \mapsto F_\infty(x_1, y) : (-1, 0) \rightarrow \mathbb{R}$  is strictly monotone decreasing

$$\frac{2}{|U|} = F_\infty(x_1, Y(x_1)) \leq F_\infty(x_1, y_0) < F_\infty(x_0, y_0) = \frac{2}{|U|},$$

which is a contradiction. Thus there exists  $\varepsilon_3 \in (0, \varepsilon_1]$  such that

$$Y(x) < y_0, \quad \forall x \in (x_0 - \varepsilon_3, x_0).$$

Similarly, suppose that for any  $\varepsilon_4 \in (0, \varepsilon_1]$  there exists  $x_2 \in (x_0, x_0 + \varepsilon_4)$  such that  $Y(x_2) \leq y_0$ . By (2.20) and the monotone decreasing property of the function  $y \mapsto F_\infty(x_2, y) : (-1, 0) \rightarrow \mathbb{R}$

$$\frac{2}{|U|} = F_\infty(x_2, Y(x_2)) \geq F_\infty(x_2, y_0) > F_\infty(x_0, y_0) = \frac{2}{|U|},$$

which is again a contradiction. Therefore there exists  $\varepsilon_4 \in (0, \varepsilon_1]$  such that

$$Y(x) > y_0, \quad \forall x \in (x_0, x_0 + \varepsilon_4).$$

The above arguments conclude that the claim (2.22) holds true.

The property (2.22) implies that there exists  $\varepsilon_5 \in (0, \varepsilon_2]$  such that

$$(2.23) \quad \frac{dY}{dx}(x) > 0, \quad \forall x \in (x_0 - \varepsilon_5, x_0 + \varepsilon_5) \setminus \{x_0\}.$$

This can be confirmed by expanding the real analytic function  $Y(\cdot)$  into the Taylor series around  $x = x_0$ . By applying Lemma 2.6 again we observe that  $(x_0 - \varepsilon_5, x_0 + \varepsilon_5) \subset (0, \beta_c)$  and

$$Y(x) = \cos\left(\frac{\tau(x)}{2}\right), \quad \forall x \in (x_0 - \varepsilon_5, x_0 + \varepsilon_5).$$

We can deduce from the above equality, (2.23) and the fact  $\tau(x) \in (\pi, 2\pi)$ ,  $\forall x \in (x_0 - \varepsilon_5, x_0 + \varepsilon_5)$  that

$$\frac{d\tau}{d\beta}(\beta) < 0, \quad \forall \beta \in (x_0 - \varepsilon_5, x_0 + \varepsilon_5) \setminus \{x_0\}.$$

This combined with (2.21) concludes that  $x_0$  is a falling SPI of  $\tau(\cdot)$ .  $\square$

Let us prepare a key lemma to prove existence of a SPI of  $\tau(\cdot)$  in Subsection 2.4, Subsection 2.5 under the assumption  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$ . Let us recall the definition of the functions  $W : \mathbb{R}_{>0} \times (-1, 0) \times \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ ,  $\widehat{W} : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$  given in [25, (2.62), Proof of Proposition 2.16].

$$(2.24) \quad \begin{aligned} W(x, y, z, s) &:= \frac{\sinh(x)}{y + \cosh(x)} + s \frac{\sinh(zx)}{(y + \cosh(zx))z}, \\ \widehat{W}(x, z, s) &:= \frac{x}{1 + \frac{x^2}{2}} + s \frac{x}{1 + z^2 \frac{x^2}{2}}. \end{aligned}$$

**Lemma 2.9.** *For any  $d, b \in \mathbb{N}$ , basis  $(\hat{\mathbf{v}}_j)_{j=1}^d$  of  $\mathbb{R}^d$ ,  $e_{max}, e_{min} \in \mathbb{R}_{>0}$  satisfying  $0 < e_{min} < e_{max}$ ,  $s_0 \in (0, 1)$  there exists*

$$\{E_{s,\delta}\}_{s \in (0, s_0), \delta \in (0, 1 - s_0^{\frac{1}{d}})} \subset \mathcal{E}(e_{min}, e_{max})$$

such that if we define  $F_\delta : \mathbb{R}_{>0} \times (-1, 0) \times (0, s_0) \rightarrow \mathbb{R}$  by

$$(2.25) \quad F_\delta(x, y, s) := D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr} \left( \frac{\sinh(xE_{s,\delta}(\mathbf{k}))}{(y + \cosh(xE_{s,\delta}(\mathbf{k})))E_{s,\delta}(\mathbf{k})} \right)$$

for  $\delta \in (0, 1 - s_0^{\frac{1}{d}})$ , the following statements hold true.

(i) For any  $\delta \in (0, 1 - s_0^{\frac{1}{d}})$

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

is constant with  $s \in (0, s_0)$ .

(ii)

$$F_\delta \in C^\infty(\mathbb{R}_{>0} \times (-1, 0) \times (0, s_0)), \quad \forall \delta \in (0, 1 - s_0^{\frac{1}{d}}).$$

$$F_\delta(\cdot, y, s) \in C^\omega(\mathbb{R}_{>0}), \quad \forall (y, s) \in (-1, 0) \times (0, s_0), \quad \delta \in (0, 1 - s_0^{\frac{1}{d}}).$$

(iii)

$$\lim_{\substack{\delta \searrow 0 \\ \delta \in (0, 1 - s_0^{\frac{1}{d}})}} \frac{\partial^j F_\delta}{\partial x^j}(x, y, s) = b s e_{\max}^{j-1} \frac{\partial^j W}{\partial x^j} \left( e_{\max} x, y, \frac{e_{\min}}{e_{\max}}, \frac{1-s}{s} \right)$$

locally uniformly with  $(x, y, s)$  in  $\mathbb{R}_{>0} \times (-1, 0) \times (0, s_0)$  for  $j \in \{0, 1, 2\}$ .

(iv)

$$\begin{aligned} & \lim_{\substack{(y, \delta) \rightarrow (-1, 0) \\ (y, \delta) \in (-1, 0) \times (0, 1 - s_0^{\frac{1}{d}})}} (y+1)^{\frac{1}{2}(j+1)} \frac{\partial^j F_\delta}{\partial x^j}(\sqrt{y+1}x, y, s) \\ &= b s e_{\max}^{j-1} \frac{\partial^j \widehat{W}}{\partial x^j} \left( e_{\max} x, \frac{e_{\min}}{e_{\max}}, \frac{1-s}{s} \right) \end{aligned}$$

locally uniformly with  $(x, s)$  in  $\mathbb{R}_{>0} \times (0, s_0)$  for  $j \in \{0, 1\}$ .

**Remark 2.10.** We will use the property (i) only to discuss the derivation of the free energy density from the many-electron system in Remark 2.13. The property (i) is not necessary to prove Theorem 1.7 and Theorem 1.8.

*Proof of Lemma 2.9.* We can construct  $E_{s,\delta} \in \mathcal{E}(e_{\min}, e_{\max})$  in a way similar to the construction of “ $E$ ” in [25, Lemma A.1]. Here let us describe the initial part of the construction in detail as it was skipped in the proof of [25, Lemma A.1]. Take any  $\delta \in \mathbb{R}_{>0}$ . Define the function  $\phi_{1,\delta} : \mathbb{R} \rightarrow \mathbb{R}$  by

$$\phi_{1,\delta}(x) := \begin{cases} e^{\frac{1}{(x+\pi\delta)x}}, & x \in (-\pi\delta, 0), \\ 0, & x \in (-\infty, -\pi\delta] \cup [0, \infty). \end{cases}$$

Observe that  $\phi_{1,\delta} \in C^\infty(\mathbb{R})$ . Define the function  $\phi_{2,\delta} : \mathbb{R} \rightarrow \mathbb{R}$  by

$$\phi_{2,\delta}(x) := \frac{\int_{-\infty}^x dt \phi_{1,\delta}(t)}{\int_{-\infty}^{\infty} dt \phi_{1,\delta}(t)}.$$

It follows that  $\phi_{2,\delta} \in C^\infty(\mathbb{R})$ . Then let us define the function  $\phi_{3,\delta} : \mathbb{R} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$  by

$$\phi_{3,\delta}(x, s) := \phi_{2,\delta}(x + \pi s^{\frac{1}{d}}).$$

Observe that  $\phi_{3,\delta} \in C^\infty(\mathbb{R} \times \mathbb{R}_{>0})$  and for any  $s \in \mathbb{R}_{>0}$

$$\begin{aligned}\phi_{3,\delta}(x, s) &= 0, \quad \forall x \in (-\infty, -\pi(\delta + s^{\frac{1}{d}})], \\ \phi_{3,\delta}(x, s) &= 1, \quad \forall x \in [-\pi s^{\frac{1}{d}}, \infty), \\ \frac{\partial}{\partial x} \phi_{3,\delta}(x, s) &> 0, \quad \forall x \in (-\pi(\delta + s^{\frac{1}{d}}), -\pi s^{\frac{1}{d}}).\end{aligned}$$

Moreover, define the function  $\phi_{4,\delta} : \mathbb{R} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$  by

$$\phi_{4,\delta}(x, s) := \begin{cases} \phi_{3,\delta}(x, s), & x \in (-\infty, 0), \\ \phi_{3,\delta}(-x, s), & x \in [0, \infty). \end{cases}$$

Observe that  $\phi_{4,\delta} \in C^\infty(\mathbb{R} \times \mathbb{R}_{>0})$  and for any  $s \in \mathbb{R}_{>0}$

$$\begin{aligned}\phi_{4,\delta}(x, s) &= 1 \text{ if } |x| \leq \pi s^{\frac{1}{d}}, \\ \phi_{4,\delta}(x, s) &= 0 \text{ if } |x| \geq \pi(\delta + s^{\frac{1}{d}}), \\ \phi_{4,\delta}(x, s) &\in (0, 1) \text{ if } \pi s^{\frac{1}{d}} < |x| < \pi(\delta + s^{\frac{1}{d}}), \\ \phi_{4,\delta}(x, s) &= \phi_{4,\delta}(-x, s), \quad \forall x \in \mathbb{R}.\end{aligned}$$

Furthermore we define the function  $\phi_\delta : \mathbb{R} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$  by

$$\phi_\delta(x, s) := (e_{\max} - e_{\min})^{\frac{1}{d}} \phi_{4,\delta}(x - \pi, s), \quad \forall (x, s) \in \mathbb{R} \times \mathbb{R}_{>0}.$$

It follows that  $\phi_\delta \in C^\infty(\mathbb{R} \times \mathbb{R}_{>0})$  and for any  $s \in \mathbb{R}_{>0}$

$$\begin{aligned}\phi_\delta(x, s) &= (e_{\max} - e_{\min})^{\frac{1}{d}} \text{ if } |x - \pi| \leq \pi s^{\frac{1}{d}}, \\ \phi_\delta(x, s) &= 0 \text{ if } |x - \pi| \geq \pi(\delta + s^{\frac{1}{d}}), \\ \phi_\delta(x, s) &\in (0, (e_{\max} - e_{\min})^{\frac{1}{d}}) \text{ if } \pi s^{\frac{1}{d}} < |x - \pi| < \pi(\delta + s^{\frac{1}{d}}), \\ \phi_\delta(\pi + x, s) &= \phi_\delta(\pi - x, s), \quad \forall x \in \mathbb{R}.\end{aligned}$$

Moreover, for any  $n \in \mathbb{N} \cup \{0\}$ ,  $c, c_0, c_1, \dots, c_n \in \mathbb{R}$

$$(2.26) \quad \sup_{x \in \mathbb{R}} \left| c + \sum_{j=0}^n c_j \frac{\partial^j \phi_\delta}{\partial x^j}(x, s) \right| \text{ is constant with } s \in \mathbb{R}_{>0}.$$

Then by using  $\phi_\delta$  in place of “ $\phi$ ” we can construct  $E_{s,\delta}$  in the same way as the construction of “ $E$ ” in the proof of [25, Lemma A.1]. Let us sketch the construction for completeness. Let  $s_0 \in (0, 1)$ ,  $\delta \in (0, 1 - s_0^{\frac{1}{d}})$ . Define the function  $\Phi_\delta : \mathbb{R}^d \times (0, s_0) \rightarrow \mathbb{R}$  by

$$\Phi_\delta(x_1, \dots, x_d, s) := \prod_{j=1}^d \phi_\delta(x_j, s) + e_{\min}.$$

Observe that  $\Phi_\delta \in C^\infty(\mathbb{R}^d \times (0, s_0))$ ,

$$\begin{aligned}\Phi_\delta(x_1, \dots, x_d, s) &= e_{\max} \text{ if } |x_j - \pi| \leq \pi s^{\frac{1}{d}}, \quad \forall j \in \{1, \dots, d\}, \\ \Phi_\delta(x_1, \dots, x_d, s) &= e_{\min} \text{ if } \exists j \in \{1, \dots, d\} \text{ s.t. } |x_j - \pi| \geq \pi(\delta + s^{\frac{1}{d}}),\end{aligned}$$

$\Phi_\delta(x_1, \dots, x_d, s) \in (e_{\min}, e_{\max})$  otherwise.

Then we define the matrix-valued function  $\hat{E}_{s,\delta} : \Gamma_\infty^* \rightarrow \text{Mat}(b, \mathbb{C})$  by

$$\hat{E}_{s,\delta}(\mathbf{k}) := \Phi_\delta((\hat{\mathbf{v}}_1, \dots, \hat{\mathbf{v}}_d)^{-1} \mathbf{k}, s) I_b, \quad \mathbf{k} \in \Gamma_\infty^*.$$

Let  $E_{s,\delta} : \mathbb{R}^d \rightarrow \text{Mat}(b, \mathbb{C})$  be the periodic extension of  $\hat{E}_{s,\delta}$  so that

$$E_{s,\delta} \left( \mathbf{k} + \sum_{j=1}^d 2\pi m_j \hat{\mathbf{v}}_j \right) = \hat{E}_{s,\delta}(\mathbf{k}), \quad \forall \mathbf{k} \in \Gamma_\infty^*, \quad (m_j)_{j=1}^d \in \mathbb{Z}^d.$$

One can check that  $E_{s,\delta} \in \mathcal{E}(e_{\min}, e_{\max})$ . In particular the property (1.6) can be confirmed in the same way as in the proof of [25, Lemma A.1].

Take any  $m_j \in \mathbb{N} \cup \{0\}$  ( $j = 1, \dots, d$ ) with  $\sum_{j=1}^d m_j \leq d + 2$ . Set  $V := (\hat{\mathbf{v}}_1, \dots, \hat{\mathbf{v}}_d) \in \text{Mat}(d, \mathbb{R})$ . By (2.26) for any  $s \in (0, s_0)$

$$\begin{aligned} & \sup_{\mathbf{k} \in \mathbb{R}^d} \left\| \prod_{j=1}^d \frac{\partial^{m_j}}{\partial k_j^{m_j}} E_{s,\delta}(\mathbf{k}) \right\|_{b \times b} = \sup_{\hat{\mathbf{k}} \in [0, 2\pi]^d} \left\| \prod_{j=1}^d \frac{\partial^{m_j}}{\partial \hat{k}_j^{m_j}} \hat{E}_{s,\delta}(V \hat{\mathbf{k}}) \right\|_{b \times b} \\ &= \sup_{\hat{\mathbf{k}} \in \mathbb{R}^d} \left| \prod_{j=1}^d \left( \sum_{i=1}^d (V^{-1})_{i,j} \frac{\partial}{\partial \hat{k}_i} \right)^{m_j} \left( \prod_{j=1}^d \phi_\delta(\hat{k}_j, s) + e_{\min} \right) \right| \\ &= \sup_{(\hat{k}_2, \dots, \hat{k}_d) \in \mathbb{R}^{d-1}} \sup_{\hat{k}_1 \in \mathbb{R}} \left| \prod_{j=1}^d \left( \sum_{i=1}^d (V^{-1})_{i,j} \frac{\partial}{\partial \hat{k}_i} \right)^{m_j} \left( \phi_\delta \left( \hat{k}_1, \frac{s_0}{2} \right) \prod_{j=2}^d \phi_\delta(\hat{k}_j, s) + e_{\min} \right) \right| \\ &= \sup_{(\hat{k}_1, \hat{k}_3, \dots, \hat{k}_d) \in \mathbb{R}^{d-1}} \sup_{\hat{k}_2 \in \mathbb{R}} \left| \prod_{j=1}^d \left( \sum_{i=1}^d (V^{-1})_{i,j} \frac{\partial}{\partial \hat{k}_i} \right)^{m_j} \left( \prod_{l=1}^2 \phi_\delta \left( \hat{k}_l, \frac{s_0}{2} \right) \prod_{j=3}^d \phi_\delta(\hat{k}_j, s) + e_{\min} \right) \right| \\ &\vdots \\ &= \sup_{\hat{\mathbf{k}} \in \mathbb{R}^d} \left| \prod_{j=1}^d \left( \sum_{i=1}^d (V^{-1})_{i,j} \frac{\partial}{\partial \hat{k}_i} \right)^{m_j} \left( \prod_{j=1}^d \phi_\delta \left( \hat{k}_j, \frac{s_0}{2} \right) + e_{\min} \right) \right| \\ &= \sup_{\mathbf{k} \in \mathbb{R}^d} \left\| \prod_{j=1}^d \frac{\partial^{m_j}}{\partial k_j^{m_j}} E_{\frac{s_0}{2}, \delta}(\mathbf{k}) \right\|_{b \times b}, \end{aligned}$$

which implies the claim (i).

We can deduce the property (ii) from the equality

$$F_\delta(x, y, s) = b(2\pi)^{-d} \int_{[0, 2\pi]^d} d\hat{\mathbf{k}} \frac{\sinh(x\Phi_\delta(\hat{\mathbf{k}}, s))}{(y + \cosh(x\Phi_\delta(\hat{\mathbf{k}}, s)))\Phi_\delta(\hat{\mathbf{k}}, s)}.$$

Let us define the function  $\Phi : \mathbb{R}^d \times (0, s_0) \rightarrow \mathbb{R}$  by

$$\Phi(x_1, \dots, x_d, s) := \begin{cases} e_{\max} & \text{if } |x_j - \pi| \leq \pi s^{\frac{1}{d}}, \quad \forall j \in \{1, \dots, d\}, \\ e_{\min} & \text{if } \exists j \in \{1, \dots, d\} \text{ s.t. } |x_j - \pi| > \pi s^{\frac{1}{d}}. \end{cases}$$

Observe that

$$\lim_{\substack{\delta \searrow 0 \\ \delta \in (0, 1 - s_0^{\frac{1}{d}})}} F_\delta(x, y, s) = b(2\pi)^{-d} \int_{[0, 2\pi]^d} d\hat{\mathbf{k}} \frac{\sinh(x\Phi(\hat{\mathbf{k}}, s))}{(y + \cosh(x\Phi(\hat{\mathbf{k}}, s)))\Phi(\hat{\mathbf{k}}, s)}$$

$$= bse_{max}^{-1} W \left( e_{max}x, y, \frac{e_{min}}{e_{max}}, \frac{1-s}{s} \right)$$

locally uniformly with  $(x, y, s)$  in  $\mathbb{R}_{>0} \times (-1, 0) \times (0, s_0)$ . One can derive an upper bound on the right-hand side of the following equality to verify the claimed locally uniform convergence.

$$\begin{aligned} F_\delta(x, y, s) - bse_{max}^{-1} W \left( e_{max}x, y, \frac{e_{min}}{e_{max}}, \frac{1-s}{s} \right) \\ = b(2\pi)^{-d} \int_{Q(\pi(\delta+s^{\frac{1}{d}})) \setminus Q(\pi s^{\frac{1}{d}})} d\hat{\mathbf{k}} \\ \cdot \left( \frac{\sinh(x\Phi_\delta(\hat{\mathbf{k}}, s))}{(y + \cosh(x\Phi_\delta(\hat{\mathbf{k}}, s)))\Phi_\delta(\hat{\mathbf{k}}, s)} - \frac{\sinh(x\Phi(\hat{\mathbf{k}}, s))}{(y + \cosh(x\Phi(\hat{\mathbf{k}}, s)))\Phi(\hat{\mathbf{k}}, s)} \right), \end{aligned}$$

where  $Q(t) := [\pi - t, \pi + t]^d$  for  $t \in (0, \pi)$ . Moreover,

$$\begin{aligned} \lim_{\substack{(y, \delta) \rightarrow (-1, 0) \\ (y, \delta) \in (-1, 0) \times (0, 1 - s_0^{\frac{1}{d}})}} \sqrt{y+1} F_\delta(\sqrt{y+1}x, y, s) &= b(2\pi)^{-d} \int_{[0, 2\pi]^d} d\hat{\mathbf{k}} \frac{x}{1 + \frac{x^2}{2}\Phi(\hat{\mathbf{k}}, s)^2} \\ &= bse_{max}^{-1} \widehat{W} \left( e_{max}x, \frac{e_{min}}{e_{max}}, \frac{1-s}{s} \right) \end{aligned}$$

locally uniformly with  $(x, s)$  in  $\mathbb{R}_{>0} \times (0, s_0)$ . The convergent properties of the derivatives of  $F_\delta$  can be confirmed similarly.  $\square$

### 2.3 Non-existence of SPI

Here we prove a proposition which ensures that the claim (iv) of Theorem 1.8 implies the claim (iii) of Theorem 1.8. In the proof we will use the function  $u : \mathbb{R}_{>0} \times [-1, 1] \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$  defined by

$$u(x, y, z) := \frac{\sinh(xz)}{(y + \cosh(xz))z}.$$

We essentially rely on [25, Lemma 2.12] to prove the next proposition.

**Proposition 2.11.** *Assume that  $\frac{e_{min}}{e_{max}} > \sqrt{17 - 12\sqrt{2}}$ . Then there exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$   $\tau(\cdot)$  has no SPI in  $(0, \beta_c)$ .*

*Proof.* Let us prove the following statement.

(2.27)

There exists  $y_0 \in (-1, 0)$  such that for any  $y \in (-1, y_0]$ ,  $E \in \mathcal{E}(e_{min}, e_{max})$  there uniquely exists  $x_0 \in \mathbb{R}_{>0}$  such that  $\frac{\partial F_\infty}{\partial x}(x_0, y) = 0$ .

If (2.27) holds, then we can apply Lemma 2.7 with  $S = \mathcal{E}(e_{min}, e_{max})$  to conclude the proof.

If  $e_{min} = e_{max}$ ,  $F_\infty(x, y) = bu(x, y, e_{max})$ . For any  $y \in (-1, 0)$ ,  $\frac{\partial F_\infty}{\partial x}(x_0, y) = 0$  if and only if  $x_0 = \frac{\cosh^{-1}(|y|^{-1})}{e_{max}}$ , where  $\cosh^{-1} : [1, \infty) \rightarrow \mathbb{R}_{\geq 0}$  is the inverse function of  $\cosh|_{\mathbb{R}_{\geq 0}}$ . Thus (2.27) holds.

Assume that  $e_{min} < e_{max}$ . Let us fix  $E \in \mathcal{E}(e_{min}, e_{max})$ . By applying Rouché's theorem one can prove that there are continuous functions  $e_j : \Gamma_\infty^* \rightarrow \mathbb{R}$  ( $j = 1, 2, \dots, b$ ) such that  $e_1(\mathbf{k}) \leq e_2(\mathbf{k}) \leq \dots \leq e_b(\mathbf{k})$ ,  $\{\text{eigenvalues of } E(\mathbf{k})\} = \{e_j(\mathbf{k})\}_{j=1}^b$  for any  $\mathbf{k} \in \Gamma_\infty^*$ . It follows that

$$(2.28) \quad e_{min} = \min_{\mathbf{k} \in \Gamma_\infty^*} \min_{j \in \{1, \dots, b\}} |e_j(\mathbf{k})|, \quad e_{max} = \max_{\mathbf{k} \in \Gamma_\infty^*} \max_{j \in \{1, \dots, b\}} |e_j(\mathbf{k})|,$$

$$F_\infty(x, y) = \sum_{j=1}^b D_d \int_{\Gamma_\infty^*} d\mathbf{k} u(x, y, |e_j(\mathbf{k})|), \quad \forall (x, y) \in \mathbb{R}_{>0} \times (-1, 0),$$

$$(2.29) \quad \begin{aligned} \frac{\partial F_\infty}{\partial x}(x, y) &> 0, \quad \forall x \in \left(0, \frac{\cosh^{-1}(|y|^{-1})}{e_{max}}\right], \\ \frac{\partial F_\infty}{\partial x}(x, y) &< 0, \quad \forall x \in \left[\frac{\cosh^{-1}(|y|^{-1})}{e_{min}}, \infty\right), \quad y \in (-1, 0). \end{aligned}$$

The inequalities (2.29) imply that for any  $y \in (-1, -\frac{1}{2}]$  there exists  $x_0(y) \in (\frac{\cosh^{-1}(|y|^{-1})}{e_{max}}, \frac{\cosh^{-1}(|y|^{-1})}{e_{min}})$  such that  $\frac{\partial F_\infty}{\partial x}(x_0(y), y) = 0$ . Observe that

$$(2.30) \quad \left| \frac{e_0}{\sqrt{y+1}} x_0(y) \right| \leq c_{max} \frac{e_{max}}{e_{min}}, \quad \forall e_0 \in [e_{min}, e_{max}],$$

where

$$c_{max} := \sup_{y \in (-1, -\frac{1}{2}]} \frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}}.$$

Using the equality

$$(2.31) \quad \cosh^{-1}(|y|^{-1}) = \log \left( |y|^{-1} + \sqrt{|y|^{-2} - 1} \right),$$

we can check that  $0 < c_{max} < \infty$ . By substituting  $x = \frac{e_0}{\sqrt{y+1}} x_0(y)$  and using (2.30) we can deduce from [25, Lemma 2.12] that if  $y \in (-1, -\frac{1}{2}]$  and

$$(2.32) \quad |y+1| < \frac{c_1 \frac{e_{min}}{e_{max}} ((\frac{e_{min}}{e_{max}})^2 - 17 + 12\sqrt{2})}{2 \cosh^2(2c_{max} \frac{e_{min}}{e_{max}}) \cosh^2(c_{max} \frac{e_{min}}{e_{max}})},$$

then

$$(2.33) \quad \begin{aligned} \frac{\partial u}{\partial x}(x_0(y), y, e_0) \frac{\partial^2 u}{\partial x^2}(x_0(y), y, e_{min}) - \frac{\partial^2 u}{\partial x^2}(x_0(y), y, e_0) \frac{\partial u}{\partial x}(x_0(y), y, e_{min}) &> 0, \\ \forall e_0 \in (e_{min}, e_{max}], \end{aligned}$$

where  $c_1 \in \mathbb{R}_{>0}$  is the generic constant independent of any parameter, introduced in [25, Lemma 2.12]. We emphasize that  $c_1$  is independent of  $E$ . We can derive from (2.28), (2.33) that

$$\frac{\partial u}{\partial x}(x_0(y), y, e_{min}) \frac{\partial^2 F_\infty}{\partial x^2}(x_0(y), y) < \frac{\partial F_\infty}{\partial x}(x_0(y), y) \frac{\partial^2 u}{\partial x^2}(x_0(y), y, e_{min}) = 0.$$

Since  $\frac{\partial u}{\partial x}(x_0(y), y, e_{min}) > 0$ ,  $\frac{\partial^2 F_\infty}{\partial x^2}(x_0(y), y) < 0$ . Essentially we have proved that if  $y \in (-1, -\frac{1}{2}]$  satisfies (2.32) and  $x_0 \in (\frac{\cosh^{-1}(|y|^{-1})}{e_{max}}, \frac{\cosh^{-1}(|y|^{-1})}{e_{min}})$  satisfies  $\frac{\partial F_\infty}{\partial x}(x_0, y) = 0$ , then  $\frac{\partial^2 F_\infty}{\partial x^2}(x_0, y) < 0$ . Take any  $y \in (-1, -\frac{1}{2}]$  satisfying (2.32). Set

$$M := \left\{ x \in \left( \frac{\cosh^{-1}(|y|^{-1})}{e_{max}}, \frac{\cosh^{-1}(|y|^{-1})}{e_{min}} \right) \mid \frac{\partial F_\infty}{\partial x}(x, y) = 0 \right\}.$$

We have already seen that  $M \neq \emptyset$ . Suppose that  $\#M \geq 2$ . Since  $x \mapsto \frac{\partial F_\infty}{\partial x}(x, y) : \mathbb{R}_{>0} \rightarrow \mathbb{R}$  is real analytic, not identically zero, there exist  $x_1, x_2 \in M$  such that  $x_1 < x_2$  and  $x \notin M$  for any  $x \in (x_1, x_2)$ . However, the property  $\frac{\partial^2 F_\infty}{\partial x^2}(x_j, y) < 0$  ( $j = 1, 2$ ) implies that there exists  $x_3 \in (x_1, x_2)$  such that  $x_3 \in M$ , which is a contradiction. Therefore  $\#M = 1$ . Combined with (2.29), the above argument ensures that the claim (2.27) holds with  $y_0 = \min\{-\frac{1}{2}, -1 + \frac{c_2}{2}\}$ , where  $c_2 (\in \mathbb{R}_{>0})$  is the right-hand side of (2.32). Lemma 2.7 concludes the proof.  $\square$

## 2.4 Existence of SPI: non-critical case

Our purpose here is to prove existence of a SPI under the condition  $\frac{e_{min}}{e_{max}} < \sqrt{17 - 12\sqrt{2}}$ , or more precisely the following proposition. Remind us that the set  $\{E_{s,\delta}\}_{s \in (0, s_0), \delta \in (0, 1 - s_0^{\frac{1}{d}})} \subset \mathcal{E}(e_{min}, e_{max})$  is constructed in Lemma 2.9.

**Proposition 2.12.** *Assume that  $\frac{e_{min}}{e_{max}} < \sqrt{17 - 12\sqrt{2}}$ . Then there exist  $s_0 \in (0, 1)$  and  $\delta \in (0, 1 - s_0^{\frac{1}{d}})$  such that the following statements hold.*

- (i) *For any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $\xi \in \{r, f\}$  there exist  $U \in [-U_0, 0)$ ,  $s \in (0, s_0)$  such that  $(SPI)_\xi$  holds with  $U$  and  $E_{s,\delta} (\in \mathcal{E}(e_{min}, e_{max}))$ .*
- (ii) *For any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$  there exist  $U \in [-U_0, 0)$ ,  $s \in (0, s_0)$ ,  $n \in 4\mathbb{N} + 2$  such that  $(PT)_{n,(\rho,\eta)}$  holds with  $U$  and  $E_{s,\delta} (\in \mathcal{E}(e_{min}, e_{max}))$ .*

**Remark 2.13.** The free energy density  $F_E(\beta, t)$  was derived from the many-electron system in [25, Theorem 1.3 (ii)] for any  $E \in \mathcal{E}(e_{min}, e_{max})$ ,  $U \in \mathbb{R}_{<0}$  satisfying (1.9). It is not trivial if  $(U, E_{s,\delta})$  introduced in Proposition 2.12 (i), (ii) satisfies (1.9). If so, the existence of SPI and HOPT is guaranteed by the proposition while the derivation of the free energy density is justified by [25, Theorem 1.3 (ii)]. According to the proof of Proposition 2.12, the choice of  $s \in (0, s_0)$  depends on  $U_0$ . However, Lemma 2.9 (i) states that (1.10) with  $E = E_{s,\delta}$  is independent of  $s$ . Assume  $\frac{e_{min}}{e_{max}} < \sqrt{17 - 12\sqrt{2}}$  and let  $s_0 \in (0, 1)$ ,  $\delta \in (0, 1 - s_0^{\frac{1}{d}})$  be those introduced in Proposition 2.12. It follows in particular that

$$((1.10) \text{ with } E = E_{s,\delta}) = ((1.10) \text{ with } E = E_{\frac{s_0}{2}, \delta})$$

for any  $s \in (0, s_0)$ . Take any

$$U_0 \in \left( 0, \frac{2c'}{b} \min\{e_{min}, e_{min}^{d+1}\} \right),$$

where  $c' \in (0, 1]$  is introduced in [25, Theorem 1.3] and depends only on  $d$ ,  $b$ ,  $(\hat{\mathbf{v}}_j)_{j=1}^d$  and (1.10) with  $E = E_{\frac{s_0}{2}, \delta}$ . Then the following statements hold true.

- For any  $\xi \in \{r, f\}$  there exist  $U \in [-U_0, 0)$ ,  $s \in (0, s_0)$  such that  $(\text{SPI})_\xi$  holds and  $F_E(\beta, t)$  is derived from the many-electron system by [25, Theorem 1.3 (ii)] with  $U$  and  $E_{s,\delta}$ .
- For any  $(\rho, \eta) \in \{(+, -), (-, +)\}$  there exist  $U \in [-U_0, 0)$ ,  $s \in (0, s_0)$ ,  $n \in 4\mathbb{N} + 2$  such that  $(\text{PT})_{n,(\rho,\eta)}$  holds and  $F_E(\beta, t)$  is derived from the many-electron system by [25, Theorem 1.3 (ii)] with  $U$  and  $E_{s,\delta}$ .

Throughout this subsection we assume that  $\frac{e_{\min}}{e_{\max}} < \sqrt{17 - 12\sqrt{2}}$ . We need to introduce a function in order to construct the proof of the above proposition. Let us set the convergent power series  $p(x, y, z)$  ( $x, y, z \in \mathbb{C}$ ) by

$$p(x, y, z) := \sum_{n=1}^{\infty} \frac{(y+1)^{n-1}}{(2n)!} 2^n z^n x^n.$$

The function  $\tilde{w}(x, y, z)$  is defined in the open set  $\tilde{D}$  of  $\mathbb{C}^3$  as follows.

$$\begin{aligned} \tilde{D} &:= \{(x, y, z) \in \mathbb{C}^3 \mid |1 + yp(x, y, z)| |1 + p(x, y, 1)| > 0\}, \\ \tilde{w}(x, y, z) &:= -\frac{(1 + yp(x, y, 1))(1 + p(x, y, z))^2}{(1 + yp(x, y, z))(1 + p(x, y, 1))^2}. \end{aligned}$$

In fact in [25, Subsection 2.2] the function  $\tilde{w}$  was introduced as an analytic continuation of the function  $w : D \rightarrow \mathbb{R}$  defined by

$$\begin{aligned} (2.34) \quad w(x, y, z) &:= -\frac{(1 + y \cosh(\sqrt{y+1}\sqrt{2x}))(y + \cosh(\sqrt{y+1}\sqrt{2zx}))^2}{(1 + y \cosh(\sqrt{y+1}\sqrt{2zx}))(y + \cosh(\sqrt{y+1}\sqrt{2x}))^2}, \\ D &:= \left\{ (x, y, z) \in \mathbb{R}_{>0} \times (-1, 0) \times \mathbb{R}_{>0} \mid x < \frac{1}{2z(y+1)} (\cosh^{-1}(|y|^{-1}))^2 \right\}. \end{aligned}$$

Here we presented the full definition of these functions in order to make clear the continuity from the previous construction [25, Section 2]. The function  $w$  will be recalled in Subsection 2.5.

Set  $\eta := (\frac{e_{\min}}{e_{\max}})^2$  ( $\in (0, 17 - 12\sqrt{2})$ ). Here we only need to use the function  $x \mapsto \tilde{w}(x, -1, \eta) : (0, \eta^{-1}) \rightarrow \mathbb{R}$ , which is characterized as

$$\tilde{w}(x, -1, \eta) = \frac{(x-1)(1+\eta x)^2}{(1-\eta x)(1+x)^2}, \quad x \in (0, \eta^{-1}).$$

Since  $(\frac{1+\eta}{6\eta})^2 > \frac{1}{\eta}$ , we can define the real numbers  $a_+(\eta)$ ,  $a_-(\eta)$  by

$$a_+(\eta) := \frac{1+\eta}{6\eta} + \left( \left( \frac{1+\eta}{6\eta} \right)^2 - \frac{1}{\eta} \right)^{\frac{1}{2}}, \quad a_-(\eta) := \frac{1+\eta}{6\eta} - \left( \left( \frac{1+\eta}{6\eta} \right)^2 - \frac{1}{\eta} \right)^{\frac{1}{2}}.$$

The behavior of the function  $\tilde{w}(\cdot, -1, \eta)$  is the most important information to prove Proposition 2.12 and is summarized in [25, Lemma 2.18]. Here we restate it for readability of the present paper.

$$\begin{aligned} (2.35) \quad 1 &< a_-(\eta) < a_+(\eta) < \eta^{-1}, \\ \frac{\partial \tilde{w}}{\partial x}(x, -1, \eta) &> 0, \quad \forall x \in (0, a_-(\eta)), \end{aligned}$$

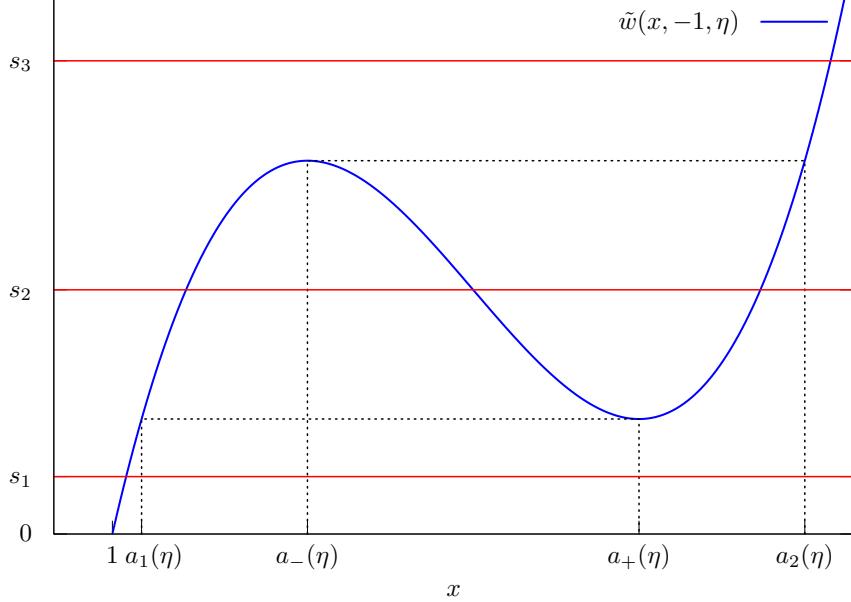


Figure 3: The schematic profile of  $\tilde{w}(\cdot, -1, \eta)$  in  $[1, \eta^{-1}]$ .

$$(2.36) \quad \frac{\partial \tilde{w}}{\partial x}(a_-(\eta), -1, \eta) = 0,$$

$$\frac{\partial \tilde{w}}{\partial x}(x, -1, \eta) < 0, \quad \forall x \in (a_-(\eta), a_+(\eta)),$$

$$(2.37) \quad \frac{\partial \tilde{w}}{\partial x}(a_+(\eta), -1, \eta) = 0,$$

$$\frac{\partial \tilde{w}}{\partial x}(x, -1, \eta) > 0, \quad \forall x \in (a_+(\eta), \eta^{-1}),$$

$$(2.38) \quad 0 < \tilde{w}(a_+(\eta), -1, \eta) < \tilde{w}(a_-(\eta), -1, \eta).$$

Since  $\tilde{w}(1, -1, \eta) = 0$  and  $\lim_{x \nearrow \eta^{-1}} \tilde{w}(x, -1, \eta) = +\infty$ , there uniquely exist  $a_1(\eta) \in (1, a_-(\eta))$ ,  $a_2(\eta) \in (a_+(\eta), \eta^{-1})$  such that

$$\tilde{w}(a_1(\eta), -1, \eta) = \tilde{w}(a_+(\eta), -1, \eta), \quad \tilde{w}(a_2(\eta), -1, \eta) = \tilde{w}(a_-(\eta), -1, \eta).$$

In the following we fix

$$\begin{aligned} s_1 &\in (0, \tilde{w}(a_+(\eta), -1, \eta)), \quad s_2 \in (\tilde{w}(a_+(\eta), -1, \eta), \tilde{w}(a_-(\eta), -1, \eta)), \\ s_3 &\in (\tilde{w}(a_-(\eta), -1, \eta), \infty). \end{aligned}$$

The schematic profile of the function  $\tilde{w}(\cdot, -1, \eta)$  in  $[1, \eta^{-1}]$  is pictured in Figure 3. We remark that Figure 3 is a sketch, not the exact implementation of  $\tilde{w}(\cdot, -1, \eta)$ .

We can prove the next lemma by combining Lemma 2.9 with the above properties of  $\tilde{w}(\cdot, -1, \eta)$ . Recall that the function  $F_\delta$  is defined in (2.25). Here we consider  $(\frac{1}{2}s_1 + 1)^{-1}$  as  $s_0$  introduced in Lemma 2.9.

**Lemma 2.14.** *There exist  $y_0 \in (-1, 0)$ ,  $\delta_0 \in (0, 1 - (\frac{1}{2}s_1 + 1)^{-\frac{1}{d}})$  such that the following statements hold for any  $y \in (-1, y_0]$ ,  $\delta \in (0, \delta_0]$ .*

(i)

$$\begin{aligned} \sqrt{2} &< \frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}} < \sqrt{2a_1(\eta)} < \sqrt{2a_-(\eta)} < \sqrt{2a_+(\eta)} < \sqrt{2a_2(\eta)} < \sqrt{2\eta^{-1}} \\ &< \sqrt{\eta^{-1}} \frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}}. \end{aligned}$$

(ii)

$$(2.39) \quad \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} x, y, \frac{1}{s_3+1} \right) > 0, \quad \forall x \in [\sqrt{2a_1(\eta)}, \sqrt{2a_+(\eta)}].$$

(2.40)

$$\begin{aligned} \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} \sqrt{2a_1(\eta)}, y, \frac{1}{s+1} \right) &> 0, \quad \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} \sqrt{2a_+(\eta)}, y, \frac{1}{s+1} \right) > 0, \\ \forall s &\in [s_2, s_3]. \end{aligned}$$

(2.41)

$$\frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} \sqrt{2a_-(\eta)}, y, \frac{1}{s_2+1} \right) < 0.$$

(iii)

$$(2.42) \quad \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} x, y, \frac{1}{s_1+1} \right) < 0, \quad \forall x \in [\sqrt{2a_-(\eta)}, \sqrt{2a_2(\eta)}].$$

(2.43)

$$\begin{aligned} \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} \sqrt{2a_-(\eta)}, y, \frac{1}{s+1} \right) &< 0, \quad \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} \sqrt{2a_2(\eta)}, y, \frac{1}{s+1} \right) < 0, \\ \forall s &\in [s_1, s_2]. \end{aligned}$$

(2.44)

$$\frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} \sqrt{2a_+(\eta)}, y, \frac{1}{s_2+1} \right) > 0.$$

*Proof.* We can derive from (2.31) that

$$(2.45) \quad \lim_{y \searrow -1} \frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}} = \sqrt{2}.$$

It was remarked in the beginning of the proof of [25, Lemma 2.24] that for  $y \in (-1, 0)$  sufficiently close to  $-1$ ,

$$(2.46) \quad \frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}} > \sqrt{2}.$$

The claim (i) follows from (2.35), (2.45), (2.46) and that  $a_1(\eta) \in (1, a_-(\eta))$ ,  $a_2(\eta) \in (a_+(\eta), \eta^{-1})$ . Recall the definition (2.24). Observe that

$$\frac{\partial \widehat{W}}{\partial x}(x, \sqrt{\eta}, s) = \frac{1 - \eta \frac{x^2}{2}}{(1 + \eta \frac{x^2}{2})^2} \left( s - \tilde{w} \left( \frac{x^2}{2}, -1, \eta \right) \right), \quad \forall (x, s) \in (0, \sqrt{2\eta^{-1}}) \times \mathbb{R}_{>0},$$

and thus by (2.38) and the choice of  $s_1, s_2, s_3$

$$\begin{aligned}
(2.47) \quad & \frac{\partial \widehat{W}}{\partial x}(x, \sqrt{\eta}, s_3) > 0, \quad \forall x \in [\sqrt{2a_1(\eta)}, \sqrt{2a_+(\eta)}]. \\
& \frac{\partial \widehat{W}}{\partial x}(\sqrt{2a_1(\eta)}, \sqrt{\eta}, s) > 0, \quad \frac{\partial \widehat{W}}{\partial x}(\sqrt{2a_+(\eta)}, \sqrt{\eta}, s) > 0, \quad \forall s \in [s_2, s_3]. \\
& \frac{\partial \widehat{W}}{\partial x}(\sqrt{2a_-(\eta)}, \sqrt{\eta}, s_2) < 0. \\
& \frac{\partial \widehat{W}}{\partial x}(x, \sqrt{\eta}, s_1) < 0, \quad \forall x \in [\sqrt{2a_-(\eta)}, \sqrt{2a_2(\eta)}]. \\
& \frac{\partial \widehat{W}}{\partial x}(\sqrt{2a_-(\eta)}, \sqrt{\eta}, s) < 0, \quad \frac{\partial \widehat{W}}{\partial x}(\sqrt{2a_2(\eta)}, \sqrt{\eta}, s) < 0, \quad \forall s \in [s_1, s_2]. \\
& \frac{\partial \widehat{W}}{\partial x}(\sqrt{2a_+(\eta)}, \sqrt{\eta}, s_2) > 0.
\end{aligned}$$

Figure 3 may help us understand the above inequalities. Lemma 2.9 (iv) implies that

$$\lim_{\substack{(y, \delta) \rightarrow (-1, 0) \\ (y, \delta) \in (-1, 0) \times (0, 1 - (\frac{1}{2}s_1 + 1)^{-\frac{1}{d}})}} (y + 1) \frac{\partial F_\delta}{\partial x} \left( \frac{\sqrt{y+1}}{e_{max}} x, y, \frac{1}{s+1} \right) = \frac{b}{s+1} \frac{\partial \widehat{W}}{\partial x}(x, \sqrt{\eta}, s)$$

uniformly with  $(x, s)$  in  $[\sqrt{2a_1(\eta)}, \sqrt{2a_2(\eta)}] \times [s_1, s_3]$ . We can deduce the claims (ii), (iii) by combining the above convergent property with (2.47).  $\square$

The proof of Proposition 2.12 is based on Corollary 2.5, Lemma 2.8, Lemma 2.9 and Lemma 2.14.

*Proof of Proposition 2.12.* By Corollary 2.5 the claim (i) is equivalent to the claim (ii). Thus it suffices to give a proof to the claim (i). Let  $y_0 \in (-1, 0)$ ,  $\delta_0 \in (0, 1 - (\frac{1}{2}s_1 + 1)^{-\frac{1}{d}})$  be those introduced in Lemma 2.14. Observe that for any  $x \in [\sqrt{2a_1(\eta)}, \sqrt{2a_2(\eta)}]$ ,  $s \in [s_1, s_3]$ ,  $\delta \in (0, \delta_0]$

$$\begin{aligned}
& \sqrt{y+1} F_\delta \left( \frac{\sqrt{y+1}}{e_{max}} x, y, \frac{1}{s+1} \right) \\
& \geq \frac{b}{(s_3+1)e_{max}} \inf_{\substack{x' \in [\sqrt{2a_1(\eta)}, \sqrt{2a_2(\eta)}] \\ s' \in [s_1, s_3]}} \widehat{W}(x', \sqrt{\eta}, s') \\
& \quad - \sup_{\substack{x' \in [\sqrt{2a_1(\eta)}, \sqrt{2a_2(\eta)}] \\ s' \in [s_1, s_3]}} \left| \sqrt{y+1} F_\delta \left( \frac{\sqrt{y+1}}{e_{max}} x', y, \frac{1}{s'+1} \right) - \frac{b}{(s'+1)e_{max}} \widehat{W}(x', \sqrt{\eta}, s') \right|.
\end{aligned}$$

We can apply Lemma 2.9 (iv) to ensure that there exist  $y_1 \in (-1, y_0]$ ,  $\delta_1 \in (0, \delta_0]$  such that

$$F_{\delta_1} \left( \frac{\sqrt{y+1}}{e_{max}} x, y, \frac{1}{s+1} \right) \geq \frac{b}{2\sqrt{y+1}(s_3+1)e_{max}} \inf_{\substack{x' \in [\sqrt{2a_1(\eta)}, \sqrt{2a_2(\eta)}] \\ s' \in [s_1, s_3]}} \widehat{W}(x', \sqrt{\eta}, s')$$

for any  $y \in (-1, y_1]$ . Take any  $U_0 \in (0, \frac{2e_{max}}{b})$ . By the above inequality there exists  $y_2 \in (-1, y_1]$  such that

$$(2.48) \quad F_{\delta_1} \left( \frac{\sqrt{y_2+1}}{e_{max}} x, y_2, \frac{1}{s+1} \right) \geq \frac{2}{U_0}, \quad \forall x \in [\sqrt{2a_1(\eta)}, \sqrt{2a_2(\eta)}], \quad s \in [s_1, s_3].$$

Here we apply the inequalities given in Lemma 2.14 (ii) with  $\delta = \delta_1$ ,  $y = y_2$ . By (2.39), (2.41) and the fact that  $s \mapsto \min_{x \in I} \frac{\partial F_{\delta_1}}{\partial x}(x, y_2, \frac{1}{s+1})$  is continuous in  $[s_2, s_3]$  for any closed bounded interval  $I \subset \mathbb{R}_{>0}$  there exists  $\hat{s} \in (s_2, s_3)$  such that

$$\min_{x \in \left[ \frac{\sqrt{y_2+1}}{e_{max}} \sqrt{2a_1(\eta)}, \frac{\sqrt{y_2+1}}{e_{max}} \sqrt{2a_+(\eta)} \right]} \frac{\partial F_{\delta_1}}{\partial x} \left( x, y_2, \frac{1}{\hat{s}+1} \right) = 0.$$

Moreover, by (2.40) there exists

$$\hat{x} \in \left( \frac{\sqrt{y_2+1}}{e_{max}} \sqrt{2a_1(\eta)}, \frac{\sqrt{y_2+1}}{e_{max}} \sqrt{2a_+(\eta)} \right)$$

such that

$$\frac{\partial F_{\delta_1}}{\partial x} \left( \hat{x}, y_2, \frac{1}{\hat{s}+1} \right) = 0.$$

Furthermore, since  $x \mapsto \frac{\partial F_{\delta_1}}{\partial x}(x, y_2, \frac{1}{\hat{s}+1}) : \mathbb{R}_{>0} \rightarrow \mathbb{R}$  is real analytic and not identically zero, there exists  $\varepsilon \in \mathbb{R}_{>0}$  such that

$$\begin{aligned} (\hat{x} - \varepsilon, \hat{x} + \varepsilon) &\subset \left( \frac{\sqrt{y_2+1}}{e_{max}} \sqrt{2a_1(\eta)}, \frac{\sqrt{y_2+1}}{e_{max}} \sqrt{2a_+(\eta)} \right), \\ \frac{\partial F_{\delta_1}}{\partial x} \left( x, y_2, \frac{1}{\hat{s}+1} \right) &> 0, \quad \forall x \in (\hat{x} - \varepsilon, \hat{x} + \varepsilon) \setminus \{\hat{x}\}. \end{aligned}$$

This means that  $\hat{x}$  is a rising SPI of  $F_{\delta_1}(\cdot, y_2, \frac{1}{\hat{s}+1})$ . Since  $F_{\delta_1}(\cdot, y_2, \frac{1}{\hat{s}+1}) = F_{\infty}(\cdot, y_2)$  with  $E_{\frac{1}{\hat{s}+1}, \delta_1} \in \mathcal{E}(e_{min}, e_{max})$ , the above property and (2.48) enable us to apply Lemma 2.8 (i) to conclude that there exists  $U \in [-U_0, 0)$  such that  $\tau(\cdot)$  has a falling SPI in  $(0, \beta_c)$ .

Using Lemma 2.14 (iii), Lemma 2.8 (ii) in place of Lemma 2.14 (ii), Lemma 2.8 (i) respectively, we can argue in a way parallel to the above argument to prove existence of a rising SPI of  $\tau(\cdot)$  for some  $U \in [-U_0, 0)$ ,  $E_{\frac{1}{\hat{s}+1}, \delta_1} \in \mathcal{E}(e_{min}, e_{max})$  with  $\tilde{s} \in (s_1, s_2)$ .

We have proved the claims with  $s_0 = (\frac{1}{2}s_1 + 1)^{-1}$ ,  $\delta = \delta_1$ .  $\square$

## 2.5 Existence of SPI: critical case

Here we prove existence of a SPI when  $\frac{e_{min}}{e_{max}} = \sqrt{17 - 12\sqrt{2}}$ .

**Proposition 2.15.** *Assume that  $\frac{e_{min}}{e_{max}} = \sqrt{17 - 12\sqrt{2}}$ . Then the following statements hold.*

- (i) *For any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $\xi \in \{r, f\}$  there exist  $U \in [-U_0, 0)$ ,  $s \in (0, 1)$ ,  $\delta \in (0, 1 - s^{\frac{1}{d}})$  such that  $(SPI)_{\xi}$  holds with  $U$  and  $E_{s, \delta} (\in \mathcal{E}(e_{min}, e_{max}))$ .*
- (ii) *For any  $U_0 \in (0, \frac{2e_{min}}{b})$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$  there exist  $U \in [-U_0, 0)$ ,  $s \in (0, 1)$ ,  $\delta \in (0, 1 - s^{\frac{1}{d}})$ ,  $n \in 4\mathbb{N} + 2$  such that  $(PT)_{n, (\rho, \eta)}$  holds with  $U$  and  $E_{s, \delta} (\in \mathcal{E}(e_{min}, e_{max}))$ .*

**Remark 2.16.** As we can see from the proof, we have to choose  $s \in (0, 1)$ ,  $\delta \in (0, 1 - s^{\frac{1}{d}})$  after fixing  $U_0$ . We cannot prove that the condition (1.9) holds for the pair  $(U, E_{s,\delta})$  introduced in the proposition. Accordingly we cannot prove existence of a SPI of  $\tau(\cdot) : (0, \beta_c) \rightarrow \mathbb{R}$  or existence of a HOPT driven by temperature while justifying the derivation of  $F_E(\beta, t)$  from the many-electron system in the case  $\frac{e_{min}}{e_{max}} = \sqrt{17 - 12\sqrt{2}}$ . In the case  $\frac{e_{min}}{e_{max}} < \sqrt{17 - 12\sqrt{2}}$  we can choose  $\delta$  before fixing  $U_0$  as claimed in Proposition 2.12, and thus we can reach the positive conclusions stated in Remark 2.13.

Set  $\eta_0 := 17 - 12\sqrt{2}$ ,  $a_0 := 3 + 2\sqrt{2}$ . As a preliminary, let us recall properties of the function

$$\tilde{w}(x, -1, \eta_0) = \frac{(x-1)(1+\eta_0x)^2}{(1-\eta_0x)(1+x)^2}, \quad x \in (0, \eta_0^{-1}),$$

which form the basis of the proof. Observe that

$$\frac{\partial \tilde{w}}{\partial x}(x, -1, \eta_0) = \frac{3\eta_0(1-\eta_0)(1+\eta_0x)}{(1-\eta_0x)^2(1+x)^3} \left( x^2 - \frac{\eta_0+1}{3\eta_0}x + \frac{1}{\eta_0} \right),$$

which is equal to [25, (2.47)], and

$$x^2 - \frac{\eta_0+1}{3\eta_0}x + \frac{1}{\eta_0} = (x - a_0)^2.$$

These imply that

$$(2.49) \quad \begin{aligned} \frac{\partial \tilde{w}}{\partial x}(x, -1, \eta_0) &> 0, \quad \forall x \in (0, \eta_0^{-1}) \setminus \{a_0\}, \\ \frac{\partial \tilde{w}}{\partial x}(a_0, -1, \eta_0) &= 0, \end{aligned}$$

and thus

$$(2.50) \quad \begin{aligned} \frac{1}{2}\tilde{w}(a_0, -1, \eta_0) &< \tilde{w}(a_0, -1, \eta_0) < \tilde{w}\left(\frac{1}{2}\eta_0^{-1}, -1, \eta_0\right), \\ \sup_{x \in [1, a_0]} \tilde{w}(x, -1, \eta_0) &< 2\tilde{w}(a_0, -1, \eta_0), \\ \inf_{x \in [a_0, \frac{1}{2}\eta_0^{-1}]} \tilde{w}(x, -1, \eta_0) &> \frac{1}{2}\tilde{w}(a_0, -1, \eta_0). \end{aligned}$$

In the proof of Proposition 2.15 we essentially use [25, Lemma 2.15], which concerns properties of the function  $w(x, y, \eta_0)$  defined in (2.34).

*Proof of Proposition 2.15.* By Corollary 2.5 the claim (i) is equivalent to the claim (ii). Thus it suffices to prove the claim (i). We apply Lemma 2.9 (iv) with  $s_0 = (1 + \frac{1}{3}\tilde{w}(a_0, -1, \eta_0))^{-1}$  to ensure that there exist  $\delta_1 \in (0, 1 - (1 + \frac{1}{3}\tilde{w}(a_0, -1, \eta_0))^{-\frac{1}{d}})$ ,  $y_1 \in (-1, 0)$  such that

$$\begin{aligned} &\sqrt{y+1}F_\delta\left(\frac{\sqrt{y+1}}{e_{max}}x, y, \frac{1}{s+1}\right) \\ &\geq \frac{b}{2(2\tilde{w}(a_0, -1, \eta_0) + 1)e_{max}} \inf_{x' \in [\sqrt{2}, \sqrt{2\eta_0^{-1}}]} \widehat{W}\left(x', \sqrt{\eta_0}, \frac{1}{2}\tilde{w}(a_0, -1, \eta_0)\right), \end{aligned}$$

$$\forall x \in [\sqrt{2}, \sqrt{2\eta_0^{-1}}], \ y \in (-1, y_1], \ s \in \left[ \frac{1}{2}\tilde{w}(a_0, -1, \eta_0), 2\tilde{w}(a_0, -1, \eta_0) \right], \ \delta \in (0, \delta_1].$$

Take any  $U_0 \in (0, \frac{2e_{min}}{b})$ . The above property guarantees that there exists  $y_2 \in (-1, y_1]$  such that

(2.51)

$$F_\delta \left( \frac{\sqrt{y+1}}{e_{max}} x, y, \frac{1}{s+1} \right) \geq \frac{2}{U_0},$$

$$\forall x \in [\sqrt{2}, \sqrt{2\eta_0^{-1}}], \ y \in (-1, y_2], \ s \in \left[ \frac{1}{2}\tilde{w}(a_0, -1, \eta_0), 2\tilde{w}(a_0, -1, \eta_0) \right], \ \delta \in (0, \delta_1].$$

It follows from [25, Lemma 2.15] that there exists  $y_3 \in (-1, y_2]$  such that for any  $y \in (-1, y_3]$

$$\begin{aligned} \frac{1}{2(y+1)}(\cosh^{-1}(|y|^{-1}))^2 &< a_0 < \frac{1}{2\eta_0(y+1)}(\cosh^{-1}(|y|^{-1}))^2, \\ 0 &< w(a_0, y, \eta_0) < 1. \end{aligned}$$

Moreover, there exist

$$x_1(y) \in \left( \frac{1}{2(y+1)}(\cosh^{-1}(|y|^{-1}))^2, a_0 \right), \ x_2(y) \in \left( a_0, \frac{1}{2\eta_0(y+1)}(\cosh^{-1}(|y|^{-1}))^2 \right)$$

such that

$$\begin{aligned} (2.52) \quad w(x_1(y), y, \eta_0) &= w(a_0, y, \eta_0) = w(x_2(y), y, \eta_0), \\ w(x, y, \eta_0) &> w(a_0, y, \eta_0), \ \forall x \in (x_1(y), a_0), \\ w(x, y, \eta_0) &< w(a_0, y, \eta_0), \ \forall x \in (a_0, x_2(y)). \end{aligned}$$

We can deduce from (2.46), (2.50) and the property

$$(2.53) \quad \lim_{y \searrow -1} \sup_{x \in [1, \frac{1}{2}\eta_0^{-1}]} |w(x, y, \eta_0) - \tilde{w}(x, -1, \eta_0)| = 0$$

that there exists  $y_4 \in (-1, y_3]$  such that

$$\begin{aligned} 1 &< \frac{1}{2(y+1)}(\cosh^{-1}(|y|^{-1}))^2, \\ \frac{1}{2}\tilde{w}(a_0, -1, \eta_0) &< w(a_0, y, \eta_0) < \tilde{w}\left(\frac{1}{2}\eta_0^{-1}, -1, \eta_0\right), \\ (2.54) \quad \sup_{x \in [1, a_0]} w(x, y, \eta_0) &< 2\tilde{w}(a_0, -1, \eta_0), \quad \inf_{x \in [a_0, \frac{1}{2}\eta_0^{-1}]} w(x, y, \eta_0) > \frac{1}{2}\tilde{w}(a_0, -1, \eta_0) \end{aligned}$$

for any  $y \in (-1, y_4]$ .

Let us prove that there exists  $\hat{y} \in (-1, y_4]$  such that

$$(2.55) \quad x_2(\hat{y}) < \frac{1}{2}\eta_0^{-1}.$$

Set  $\xi := \frac{1}{2}(\tilde{w}(\frac{1}{2}\eta_0^{-1}, -1, \eta_0) - \tilde{w}(a_0, -1, \eta_0))$ . It follows that

$$(2.56) \quad \tilde{w}(a_0, -1, \eta_0) + \xi < \tilde{w}\left(\frac{1}{2}\eta_0^{-1}, -1, \eta_0\right).$$

By (2.53) there exists  $y_5 \in (-1, y_4]$  such that

$$(2.57) \quad w(a_0, y, \eta_0) < \tilde{w}(a_0, -1, \eta_0) + \xi, \quad \forall y \in (-1, y_5].$$

Let us take  $\varepsilon \in \mathbb{R}_{>0}$  so that

$$\eta_0^{-1} - \varepsilon > \frac{1}{2}\eta_0^{-1}, \quad \frac{\eta_0^{-1} - \varepsilon - 1}{\varepsilon\eta_0(1 + \eta_0^{-1})^2} \geq \tilde{w}\left(\frac{1}{2}\eta_0^{-1}, -1, \eta_0\right).$$

We define  $T : (-1, y_5] \rightarrow \mathbb{R}$  by

$$T(y) := -\frac{1 + y \cosh(\sqrt{y+1}\sqrt{2x})}{1 + y \cosh(\sqrt{y+1}\sqrt{2\eta_0 x})} \Big|_{x=\eta_0^{-1}-\varepsilon} \cdot \frac{(y+1)^2}{(y + \cosh(\sqrt{y+1}\sqrt{2x}))^2} \Big|_{x=\frac{1}{2\eta_0(y+1)}(\cosh^{-1}(|y|^{-1}))^2}.$$

Observe that

$$\begin{aligned} \frac{1}{2(y+1)}(\cosh^{-1}(|y|^{-1}))^2 &< \eta_0^{-1} - \varepsilon < \frac{1}{2\eta_0(y+1)}(\cosh^{-1}(|y|^{-1}))^2, \\ w(x, y, \eta_0) &\geq T(y), \quad \forall x \in \left[\eta_0^{-1} - \varepsilon, \frac{1}{2\eta_0(y+1)}(\cosh^{-1}(|y|^{-1}))^2\right], \quad y \in (-1, y_5], \\ \lim_{\substack{y \searrow -1 \\ y \in (-1, y_5]}} T(y) &= \frac{\eta_0^{-1} - \varepsilon - 1}{\varepsilon\eta_0(1 + \eta_0^{-1})^2} \geq \tilde{w}\left(\frac{1}{2}\eta_0^{-1}, -1, \eta_0\right). \end{aligned}$$

These properties plus (2.56) imply that there exists  $y_6 \in (-1, y_5]$  such that

$$(2.58) \quad \begin{aligned} w(x, y, \eta_0) &\geq \tilde{w}(a_0, -1, \eta_0) + \xi, \\ \forall x \in \left[\eta_0^{-1} - \varepsilon, \frac{1}{2\eta_0(y+1)}(\cosh^{-1}(|y|^{-1}))^2\right], \quad y &\in (-1, y_6]. \end{aligned}$$

On the other hand, since

$$\lim_{\substack{y \searrow -1 \\ y \in (-1, y_6]}} \sup_{x \in [\frac{1}{2}\eta_0^{-1}, \eta_0^{-1}-\varepsilon]} |w(x, y, \eta_0) - \tilde{w}(x, -1, \eta_0)| = 0,$$

by (2.49) and (2.56) there exists  $\hat{y} \in (-1, y_6]$  such that

$$(2.59) \quad w(x, \hat{y}, \eta_0) \geq \tilde{w}(a_0, -1, \eta_0) + \xi, \quad \forall x \in \left[\frac{1}{2}\eta_0^{-1}, \eta_0^{-1} - \varepsilon\right].$$

By combining (2.57), (2.58) with (2.59) we obtain that

$$w(x, \hat{y}, \eta_0) > w(a_0, \hat{y}, \eta_0), \quad \forall x \in \left[\frac{1}{2}\eta_0^{-1}, \frac{1}{2\eta_0(\hat{y}+1)}(\cosh^{-1}(|\hat{y}|^{-1}))^2\right].$$

If  $x_2(\hat{y}) \geq \frac{1}{2}\eta_0^{-1}$ ,

$$w(x_2(\hat{y}), \hat{y}, \eta_0) > w(a_0, \hat{y}, \eta_0) = w(x_2(\hat{y}), \hat{y}, \eta_0),$$

which is a contradiction. Therefore  $x_2(\hat{y}) < \frac{1}{2}\eta_0^{-1}$ .

Let us set

$$\begin{aligned}
s_1 &:= \frac{1}{2}\tilde{w}(a_0, -1, \eta_0), \\
s_2 &:= \frac{1}{2} \left( \inf_{x \in [a_0, x_2(\hat{y})]} w(x, \hat{y}, \eta_0) + w(a_0, \hat{y}, \eta_0) \right), \\
s_3 &:= \frac{1}{2} \left( \sup_{x \in [x_1(\hat{y}), a_0]} w(x, \hat{y}, \eta_0) + w(a_0, \hat{y}, \eta_0) \right), \\
s_4 &:= 2\tilde{w}(a_0, -1, \eta_0).
\end{aligned}$$

We can see from (2.52), (2.54), (2.55) that

$$\begin{aligned}
(2.60) \quad s_1 &< \inf_{x \in [a_0, x_2(\hat{y})]} w(x, \hat{y}, \eta_0) < s_2 < w(a_0, \hat{y}, \eta_0) = w(x_1(\hat{y}), \hat{y}, \eta_0) = w(x_2(\hat{y}), \hat{y}, \eta_0) \\
&< s_3 < \sup_{x \in [x_1(\hat{y}), a_0]} w(x, \hat{y}, \eta_0) < s_4.
\end{aligned}$$

Observe that

$$(2.61) \quad \frac{\partial W}{\partial x}(\sqrt{y+1}x, y, \sqrt{z}, s) = \frac{1+y \cosh(\sqrt{z(y+1)}x)}{(y+\cosh(\sqrt{z(y+1)}x))^2} \left( s - w\left(\frac{x^2}{2}, y, z\right) \right)$$

for any  $(x, y, z) \in \mathbb{R}_{>0} \times (-1, 0) \times \mathbb{R}_{>0}$  satisfying  $x < \frac{1}{\sqrt{z(y+1)}} \cosh^{-1}(|y|^{-1})$ . Let  $\hat{x}_1 \in (x_1(\hat{y}), a_0)$ ,  $\hat{x}_2 \in (a_0, x_2(\hat{y}))$  be such that

$$(2.62) \quad w(\hat{x}_1, \hat{y}, \eta_0) = \max_{x \in [x_1(\hat{y}), a_0]} w(x, \hat{y}, \eta_0), \quad w(\hat{x}_2, \hat{y}, \eta_0) = \min_{x \in [a_0, x_2(\hat{y})]} w(x, \hat{y}, \eta_0).$$

Combination of (2.60), (2.61), (2.62) implies that

$$\begin{aligned}
&\frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}x, \hat{y}, \sqrt{\eta_0}, s_1) < 0, \quad \forall x \in [\sqrt{2a_0}, \sqrt{2x_2(\hat{y})}], \\
&\frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}\sqrt{2a_0}, \hat{y}, \sqrt{\eta_0}, s) < 0, \quad \frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}\sqrt{2x_2(\hat{y})}, \hat{y}, \sqrt{\eta_0}, s) < 0, \quad \forall s \in [s_1, s_2], \\
&\frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}\sqrt{2\hat{x}_2}, \hat{y}, \sqrt{\eta_0}, s_2) > 0, \\
&\frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}x, \hat{y}, \sqrt{\eta_0}, s_4) > 0, \quad \forall x \in [\sqrt{2x_1(\hat{y})}, \sqrt{2a_0}], \\
&\frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}\sqrt{2x_1(\hat{y})}, \hat{y}, \sqrt{\eta_0}, s) > 0, \quad \frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}\sqrt{2a_0}, \hat{y}, \sqrt{\eta_0}, s) > 0, \quad \forall s \in [s_3, s_4], \\
&\frac{\partial W}{\partial x}(\sqrt{\hat{y}+1}\sqrt{2\hat{x}_1}, \hat{y}, \sqrt{\eta_0}, s_3) < 0.
\end{aligned}$$

Here we apply Lemma 2.9 (ii), (iii) with  $s_0 = (1 + \frac{1}{3}\tilde{w}(a_0, -1, \eta_0))^{-1}$  to derive from the above inequalities that there exists  $\hat{\delta} \in (0, \delta_1]$  such that

$$\begin{aligned}
(2.63) \quad &\frac{\partial F_{\hat{\delta}}}{\partial x}(\cdot, \hat{y}, \cdot) \in C(\mathbb{R}_{>0} \times [(s_4 + 1)^{-1}, (s_1 + 1)^{-1}]), \\
&F_{\hat{\delta}}(\cdot, \hat{y}, s) \in C^\omega(\mathbb{R}_{>0}), \quad \forall s \in [(s_4 + 1)^{-1}, (s_1 + 1)^{-1}], \\
&\frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} x, \hat{y}, \frac{1}{s_1 + 1} \right) < 0, \quad \forall x \in [\sqrt{2a_0}, \sqrt{2x_2(\hat{y})}],
\end{aligned}$$

$$(2.64) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0}, \hat{y}, \frac{1}{s+1} \right) < 0, \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_2(\hat{y})}, \hat{y}, \frac{1}{s+1} \right) < 0, \quad \forall s \in [s_1, s_2],$$

$$(2.65) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2\hat{x}_2}, \hat{y}, \frac{1}{s_2+1} \right) > 0,$$

$$(2.66) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} x, \hat{y}, \frac{1}{s_4+1} \right) > 0, \quad \forall x \in [\sqrt{2x_1(\hat{y})}, \sqrt{2a_0}],$$

$$(2.67) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_1(\hat{y})}, \hat{y}, \frac{1}{s+1} \right) > 0, \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0}, \hat{y}, \frac{1}{s+1} \right) > 0, \quad \forall s \in [s_3, s_4],$$

$$(2.68) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2\hat{x}_1}, \hat{y}, \frac{1}{s_3+1} \right) < 0.$$

By (2.63), (2.65), (2.66), (2.68) and the fact that  $s \mapsto \max_{x \in I} \frac{\partial F_{\hat{\delta}}}{\partial x}(x, \hat{y}, \frac{1}{s+1})$ ,  $s \mapsto \min_{x \in I} \frac{\partial F_{\hat{\delta}}}{\partial x}(x, \hat{y}, \frac{1}{s+1})$  are continuous in  $[s_1, s_4]$  for any closed bounded interval  $I \subset \mathbb{R}_{>0}$  there exist  $\hat{s}_1 \in (s_1, s_2)$ ,  $\hat{s}_2 \in (s_3, s_4)$  such that

$$\begin{aligned} \max_{x \in \left[ \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0}, \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_2(\hat{y})} \right]} \frac{\partial F_{\hat{\delta}}}{\partial x} \left( x, \hat{y}, \frac{1}{\hat{s}_1+1} \right) &= 0, \\ \min_{x \in \left[ \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_1(\hat{y})}, \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0} \right]} \frac{\partial F_{\hat{\delta}}}{\partial x} \left( x, \hat{y}, \frac{1}{\hat{s}_2+1} \right) &= 0. \end{aligned}$$

Moreover, by (2.64), (2.67) there exist

$$\zeta_1 \in \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_1(\hat{y})}, \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0} \right), \quad \zeta_2 \in \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0}, \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_2(\hat{y})} \right)$$

such that

$$(2.69) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \zeta_2, \hat{y}, \frac{1}{\hat{s}_1+1} \right) = 0,$$

$$(2.70) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( \zeta_1, \hat{y}, \frac{1}{\hat{s}_2+1} \right) = 0.$$

Furthermore, since  $\frac{\partial F_{\hat{\delta}}}{\partial x}(\cdot, \hat{y}, \frac{1}{\hat{s}_j+1}) \in C^\omega(\mathbb{R}_{>0})$  ( $j = 1, 2$ ) and these functions are not identically zero, there exists  $\hat{\varepsilon} \in \mathbb{R}_{>0}$  such that

$$\begin{aligned} (2.71) \quad &(\zeta_1 - \hat{\varepsilon}, \zeta_1 + \hat{\varepsilon}) \subset \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_1(\hat{y})}, \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0} \right), \\ &\frac{\partial F_{\hat{\delta}}}{\partial x} \left( x, \hat{y}, \frac{1}{\hat{s}_2+1} \right) > 0, \quad \forall x \in (\zeta_1 - \hat{\varepsilon}, \zeta_1 + \hat{\varepsilon}) \setminus \{\zeta_1\}, \\ &(\zeta_2 - \hat{\varepsilon}, \zeta_2 + \hat{\varepsilon}) \subset \left( \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2a_0}, \frac{\sqrt{\hat{y}+1}}{e_{max}} \sqrt{2x_2(\hat{y})} \right), \end{aligned}$$

$$(2.72) \quad \frac{\partial F_{\hat{\delta}}}{\partial x} \left( x, \hat{y}, \frac{1}{\hat{s}_1 + 1} \right) < 0, \quad \forall x \in (\zeta_2 - \hat{\varepsilon}, \zeta_2 + \hat{\varepsilon}) \setminus \{\zeta_2\}.$$

Finally the properties (2.51), (2.69), (2.72) enable us to apply Lemma 2.8 (ii) to ensure that for  $E_{\frac{1}{\hat{s}_1+1}, \hat{\delta}}$  ( $\in \mathcal{E}(e_{min}, e_{max})$ ) and some  $U \in [-U_0, 0)$   $\tau(\cdot)$  has a rising SPI in  $(0, \beta_c)$ . Similarly by (2.51), (2.70), (2.71) we can apply Lemma 2.8 (i) to conclude that for  $E_{\frac{1}{\hat{s}_2+1}, \hat{\delta}}$  ( $\in \mathcal{E}(e_{min}, e_{max})$ ) and some  $U \in [-U_0, 0)$   $\tau(\cdot)$  has a falling SPI in  $(0, \beta_c)$ . Thus the claim (i) holds true.  $\square$

## 2.6 Proof of Theorem 1.7 and Theorem 1.8

We can complete the proof of Theorem 1.7 and Theorem 1.8 by applying Proposition 2.11, Proposition 2.12 and Proposition 2.15.

*Proof of Theorem 1.7.* The equivalence between the claim (i) and the claim (ii) was proved in Corollary 2.4 (1). By Proposition 2.12 and Proposition 2.15 the claim (iii) implies the claim (ii). If the claim (iii) does not hold, by Proposition 2.11 the claim (ii) does not hold. Therefore the claim (iii) is equivalent to the claim (ii). The proof is complete.  $\square$

*Proof of Theorem 1.8.* Corollary 2.4 (2) ensures the equivalence between the claims (i), (ii), (iii). By Proposition 2.11 the claim (iv) implies the claim (iii). It follows from Proposition 2.12, Proposition 2.15 that if the claim (iv) does not hold, the claim (iii) does not hold. Thus the claim (iv) is equivalent to the claim (iii), which concludes the proof.  $\square$

## 3 Specific models

Our main theorems are claimed for the general set of free dispersion relations  $\mathcal{E}(e_{min}, e_{max})$ . One natural question is whether HOPT occurs in a specific model belonging to  $\mathcal{E}(e_{min}, e_{max})$  by varying parameters on which the model depends. We focus on the following 2 models of  $\mathcal{E}(e_{min}, e_{max})$ .

(1) For  $d \in \mathbb{N}$ ,  $b \in \mathbb{N}_{\geq 2}$ ,  $b' \in \{1, 2, \dots, b-1\}$ , a basis  $(\hat{\mathbf{v}}_j)_{j=1}^d$  of  $\mathbb{R}^d$ ,  $e_{min}, e_{max} \in \mathbb{R}_{>0}$  with  $e_{min} \leq e_{max}$

$$E_b(\mathbf{k}) := \begin{pmatrix} e_{max} I_{b'} & 0 \\ 0 & e_{min} I_{b-b'} \end{pmatrix}, \quad \mathbf{k} \in \mathbb{R}^d.$$

(2) For  $t \in \mathbb{R}_{\geq 0}$ ,  $e_{min} \in \mathbb{R}_{>0}$

$$E_1(k) := t(\cos k + 1) + e_{min}, \quad k \in \mathbb{R}.$$

The model (1) is actually independent of the variable  $\mathbf{k}$ . It is a one-particle Hamiltonian of non-hopping multi-orbital electron. In the model (2)  $d = b = 1$ ,  $e_{max} = 2t + e_{min}$ . It is the dispersion relation of a free electron hopping between nearest neighbor sites in the 1-dimensional lattice  $\mathbb{Z}$ . In fact these models were studied in [25, Subsection 2.3] in terms of uniqueness of local minimum point of the phase boundary. Our aim here is to study these models in terms of SPI and HOPT.

By Theorem 1.8 we know that if  $|U|$  is sufficiently small and  $\frac{e_{min}}{e_{max}} > \sqrt{17 - 12\sqrt{2}}$ , the temperature-driven phase transition is of 2nd order, and thus there is no HOPT in these models. However, our main theorems do not imply existence of a HOPT in these specific models even if  $\frac{e_{min}}{e_{max}} \leq \sqrt{17 - 12\sqrt{2}}$ . It is advantageous that we can use the technical lemma [25, Lemma 2.24] to analyze the model (1). It turns out that the model (1) shows quite rich behavior in terms of SPI and HOPT, depending on  $\frac{e_{min}}{e_{max}}$  and  $\frac{b-b'}{b'}$ . Also we can deduce non-existence of SPI in the model (2) from the proof of [25, Proposition 2.26].

Concerning the model (1), we want to prove the following proposition.

**Proposition 3.1.** (i) Assume that  $\frac{b-b'}{b'} \in [3 - 2\sqrt{2}, \infty)$ . Then for any  $e_{min}, e_{max} \in \mathbb{R}_{>0}$  satisfying  $e_{min} \leq e_{max}$  there exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$   $\tau(\cdot)$  has no SPI in  $(0, \beta_c)$ .

(ii) Assume that  $\frac{b-b'}{b'} \in (\frac{1}{8}, 3 - 2\sqrt{2})$ . Then for any  $e_{min} \in \mathbb{R}_{>0}$ ,  $U_0 \in (0, \frac{2e_{min}}{b})$  there exist  $e_1, e_2 \in (0, \sqrt{17 - 12\sqrt{2}})$ ,  $U_1, U_2 \in [-U_0, 0)$  such that  $e_2 < e_1$  and if  $\frac{e_{min}}{e_{max}} = e_1$ ,  $U = U_1$ ,  $\tau(\cdot)$  has a rising SPI in  $(0, \beta_c)$ , if  $\frac{e_{min}}{e_{max}} = e_2$ ,  $U = U_2$ ,  $\tau(\cdot)$  has a falling SPI in  $(0, \beta_c)$ .

(iii) Assume that  $\frac{b-b'}{b'} \in (0, \frac{1}{8}]$ . Then for any  $e_{min} \in \mathbb{R}_{>0}$ ,  $U_0 \in (0, \frac{2e_{min}}{b})$  there exist  $e_3 \in (0, \sqrt{17 - 12\sqrt{2}})$ ,  $U \in [-U_0, 0)$  such that if  $\frac{e_{min}}{e_{max}} = e_3$ ,  $\tau(\cdot)$  has a rising SPI in  $(0, \beta_c)$ .

We can derive the following corollary from the above proposition and Theorem 1.6.

**Corollary 3.2.** (i) Assume that  $\frac{b-b'}{b'} \in [3 - 2\sqrt{2}, \infty)$ . Then for any  $e_{min}, e_{max} \in \mathbb{R}_{>0}$  satisfying  $e_{min} \leq e_{max}$  there exists  $U_0 \in (0, \frac{2e_{min}}{b})$  such that for any  $U \in [-U_0, 0)$ ,  $(\rho, \eta) \in \{(+, -), (-, +)\}$ ,  $(\beta, t) \in Q_{\rho, \eta}$   $(PT)_{2, (\rho, \eta)}(\beta, t)$  holds.

(ii) Assume that  $\frac{b-b'}{b'} \in (\frac{1}{8}, 3 - 2\sqrt{2})$ . Then for any  $e_{min} \in \mathbb{R}_{>0}$ ,  $U_0 \in (0, \frac{2e_{min}}{b})$  there exist  $e_1, e_2 \in (0, \sqrt{17 - 12\sqrt{2}})$ ,  $U_1, U_2 \in [-U_0, 0)$  such that  $e_2 < e_1$  and if  $\frac{e_{min}}{e_{max}} = e_1$ ,  $U = U_1$ ,  $(PT)_{n, (+, -)}$  holds for some  $n \in 4\mathbb{N} + 2$ , if  $\frac{e_{min}}{e_{max}} = e_2$ ,  $U = U_2$ ,  $(PT)_{n, (-, +)}$  holds for some  $n \in 4\mathbb{N} + 2$ .

(iii) Assume that  $\frac{b-b'}{b'} \in (0, \frac{1}{8}]$ . Then for any  $e_{min} \in \mathbb{R}_{>0}$ ,  $U_0 \in (0, \frac{2e_{min}}{b})$  there exist  $e_3 \in (0, \sqrt{17 - 12\sqrt{2}})$ ,  $U \in [-U_0, 0)$  such that if  $\frac{e_{min}}{e_{max}} = e_3$ ,  $(PT)_{n, (+, -)}$  holds for some  $n \in 4\mathbb{N} + 2$ .

The proof of Proposition 3.1 is based on Lemma 3.3 below. Recall the definition of the functions  $w(x, y, z)$ ,  $\tilde{w}(x, y, z)$  and their properties summarized in front of Lemma 2.14 to understand the statements and the proof of the lemma. In addition we will use the following properties.

$$(3.1) \quad \lim_{\eta \nearrow 17-12\sqrt{2}} \tilde{w}(a_+(\eta), -1, \eta) = \lim_{\eta \nearrow 17-12\sqrt{2}} \tilde{w}(a_-(\eta), -1, \eta) = 3 - 2\sqrt{2},$$

$$(3.2) \quad \lim_{\eta \searrow 0} \tilde{w}(a_-(\eta), -1, \eta) = \frac{1}{8}, \quad \lim_{\eta \searrow 0} \tilde{w}(a_+(\eta), -1, \eta) = 0,$$

which can be derived from the facts that

$$\lim_{\eta \nearrow 17-12\sqrt{2}} a_+(\eta) = \lim_{\eta \nearrow 17-12\sqrt{2}} a_-(\eta) = 3 + 2\sqrt{2},$$

$$\lim_{\eta \searrow 0} a_-(\eta) = 3, \lim_{\eta \searrow 0} a_+(\eta) = +\infty, \lim_{\eta \searrow 0} \eta a_+(\eta) = \frac{1}{3}.$$

Moreover we need that

$$(3.3) \quad \frac{d}{d\eta} \tilde{w}(a_\delta(\eta), -1, \eta) > 0, \quad \forall \delta \in \{+, -\}, \quad \eta \in (0, 17 - 12\sqrt{2}).$$

This can be confirmed as follows.

$$(3.4) \quad \frac{\partial \tilde{w}}{\partial z}(x, -1, z) = \frac{(x-1)x(1+zx)(3-zx)}{(x+1)^2(1-zx)^2} > 0, \quad \forall z \in (0, 1), \quad x \in (1, z^{-1}),$$

and thus by (2.35), (2.36), (2.37)

$$\begin{aligned} \frac{d}{d\eta} \tilde{w}(a_\delta(\eta), -1, \eta) &= \frac{\partial \tilde{w}}{\partial x}(a_\delta(\eta), -1, \eta) \frac{da_\delta}{d\eta}(\eta) + \frac{\partial \tilde{w}}{\partial z}(a_\delta(\eta), -1, \eta) \\ &= \frac{\partial \tilde{w}}{\partial z}(a_\delta(\eta), -1, \eta) > 0, \quad \forall \eta \in (0, 17 - 12\sqrt{2}), \quad \delta \in \{+, -\}. \end{aligned}$$

**Lemma 3.3.** (i) For any  $s \in (\frac{1}{8}, 3 - 2\sqrt{2})$  there exist  $\eta_1, \eta_2, \eta_3, \eta_4 \in (0, 17 - 12\sqrt{2})$ ,  $y_1 \in (-1, 0)$  such that  $\eta_4 < \eta_3 < \eta_2 < \eta_1$ ,  $a_+(\eta_2) < \eta_1^{-1}$  and for any  $y \in (-1, y_1]$

$$\frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}} > \sqrt{2},$$

$$\begin{aligned} w(x, y, \eta_1) &> s, \quad \forall x \in \left[ \frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), \frac{1}{2}(a_+(\eta_2) + \eta_1^{-1}) \right], \\ w\left(\frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), y, \eta\right) &> s, \quad w\left(\frac{1}{2}(a_+(\eta_2) + \eta_1^{-1}), y, \eta\right) > s, \quad \forall \eta \in [\eta_2, \eta_1], \\ w(a_+(\eta_2), y, \eta_2) &< s, \\ w(x, y, \eta_4) &< s, \quad \forall x \in \left[ \frac{1}{2}(1 + a_-(\eta_3)), \frac{1}{2}(a_-(\eta_3) + a_+(\eta_3)) \right], \\ w\left(\frac{1}{2}(1 + a_-(\eta_3)), y, \eta\right) &< s, \quad w\left(\frac{1}{2}(a_-(\eta_3) + a_+(\eta_3)), y, \eta\right) < s, \quad \forall \eta \in [\eta_4, \eta_3], \\ w(a_-(\eta_3), y, \eta_3) &> s. \end{aligned}$$

(ii) For any  $s \in (0, \frac{1}{8}]$  there exist  $\eta_5, \eta_6 \in (0, 17 - 12\sqrt{2})$ ,  $y_2 \in (-1, 0)$  such that  $\eta_6 < \eta_5$ ,  $a_+(\eta_6) < \eta_5^{-1}$  and for any  $y \in (-1, y_2]$

$$\frac{\cosh^{-1}(|y|^{-1})}{\sqrt{y+1}} > \sqrt{2},$$

$$\begin{aligned} w(x, y, \eta_5) &> s, \quad \forall x \in \left[ \frac{1}{2}(a_-(\eta_6) + a_+(\eta_6)), \frac{1}{2}(a_+(\eta_6) + \eta_5^{-1}) \right], \\ w\left(\frac{1}{2}(a_-(\eta_6) + a_+(\eta_6)), y, \eta\right) &> s, \quad w\left(\frac{1}{2}(a_+(\eta_6) + \eta_5^{-1}), y, \eta\right) > s, \quad \forall \eta \in [\eta_6, \eta_5], \\ w(a_+(\eta_6), y, \eta_6) &< s. \end{aligned}$$

**Remark 3.4.** By using the inequality  $\cosh^{-1}(|y|^{-1})/\sqrt{y+1} > \sqrt{2}$  we can check that the variable  $(x, y, \eta)$  belongs to the domain  $D$  where the function  $w$  is defined in the statement of the above lemma.

*Proof.* (i): Take any  $s \in (\frac{1}{8}, 3 - 2\sqrt{2})$ . We can deduce from the properties (2.38), (3.1), (3.2), (3.3) that there uniquely exist  $\hat{\eta}_1, \hat{\eta}_2 \in (0, 17 - 12\sqrt{2})$  such that  $\hat{\eta}_2 < \hat{\eta}_1$ ,

$$\tilde{w}(a_+(\hat{\eta}_1), -1, \hat{\eta}_1) = \tilde{w}(a_-(\hat{\eta}_2), -1, \hat{\eta}_2) = s.$$

Moreover, by the profile of  $\tilde{w}(\cdot, -1, \eta)$  described in Subsection 2.4, (3.3) and (3.4) there exists small  $\varepsilon \in \mathbb{R}_{>0}$  such that the following inequalities hold.

$$a_+(\hat{\eta}_1) < \hat{\eta}_1^{-1}.$$

$$\tilde{w}(x, -1, \eta) > s, \quad \forall x \in \left[ \frac{1}{2}(a_-(\hat{\eta}_1) + a_+(\hat{\eta}_1)) - \varepsilon, \frac{1}{2}(a_+(\hat{\eta}_1) + \hat{\eta}_1^{-1}) + \varepsilon \right], \quad \eta \in (\hat{\eta}_1, \hat{\eta}_1 + \varepsilon].$$

$$\tilde{w}\left(\frac{1}{2}(a_-(\hat{\eta}_1) + a_+(\hat{\eta}_1)), -1, \hat{\eta}_1\right) > s, \quad \tilde{w}\left(\frac{1}{2}(a_+(\hat{\eta}_1) + \hat{\eta}_1^{-1}), -1, \hat{\eta}_1\right) > s.$$

$$\tilde{w}(a_+(\eta), -1, \eta) < s, \quad \forall \eta \in [\hat{\eta}_1 - \varepsilon, \hat{\eta}_1].$$

$$\tilde{w}(x, -1, \eta) < s, \quad \forall x \in \left[ \frac{1}{2}(1 + a_-(\hat{\eta}_2)) - \varepsilon, \frac{1}{2}(a_-(\hat{\eta}_2) + a_+(\hat{\eta}_2)) + \varepsilon \right], \quad \eta \in [\hat{\eta}_2 - \varepsilon, \hat{\eta}_2].$$

$$\tilde{w}\left(\frac{1}{2}(1 + a_-(\hat{\eta}_2)), -1, \hat{\eta}_2\right) < s, \quad \tilde{w}\left(\frac{1}{2}(a_-(\hat{\eta}_2) + a_+(\hat{\eta}_2)), -1, \hat{\eta}_2\right) < s.$$

$$\tilde{w}(a_-(\eta), -1, \eta) > s, \quad \forall \eta \in (\hat{\eta}_2, \hat{\eta}_2 + \varepsilon].$$

Then we can choose  $\eta_1 \in (\hat{\eta}_1, 17 - 12\sqrt{2})$ ,  $\eta_2 \in (0, \hat{\eta}_1)$  to be close to  $\hat{\eta}_1$  and  $\eta_3 \in (\hat{\eta}_2, 17 - 12\sqrt{2})$ ,  $\eta_4 \in (0, \hat{\eta}_2)$  to be close to  $\hat{\eta}_2$  so that  $\eta_4 < \eta_3 < \eta_2 < \eta_1$ ,

(3.5)

$$a_+(\eta_2) < \eta_1^{-1},$$

(3.6)

$$\tilde{w}(x, -1, \eta_1) > s, \quad \forall x \in \left[ \frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), \frac{1}{2}(a_+(\eta_2) + \eta_1^{-1}) \right],$$

(3.7)

$$\tilde{w}\left(\frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), -1, \eta\right) > s, \quad \tilde{w}\left(\frac{1}{2}(a_+(\eta_2) + \eta_1^{-1}), -1, \eta\right) > s, \quad \forall \eta \in [\eta_2, \eta_1],$$

(3.8)

$$\tilde{w}(a_+(\eta_2), -1, \eta_2) < s,$$

$$\tilde{w}(x, -1, \eta_4) < s, \quad \forall x \in \left[ \frac{1}{2}(1 + a_-(\eta_3)), \frac{1}{2}(a_-(\eta_3) + a_+(\eta_3)) \right],$$

$$\tilde{w}\left(\frac{1}{2}(1 + a_-(\eta_3)), -1, \eta\right) < s, \quad \tilde{w}\left(\frac{1}{2}(a_-(\eta_3) + a_+(\eta_3)), -1, \eta\right) < s, \quad \forall \eta \in [\eta_4, \eta_3],$$

$$\tilde{w}(a_-(\eta_3), -1, \eta_3) > s.$$

The claimed inequalities follow from (2.46), the above inequalities and the uniform convergence properties

$$(3.9) \quad \lim_{y \searrow -1} \sup_{\substack{x \in [\frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), \frac{1}{2}(a_+(\eta_2) + \eta_1^{-1})] \\ \eta \in [\eta_2, \eta_1]}} |w(x, y, \eta) - \tilde{w}(x, -1, \eta)| = 0,$$

$$\lim_{y \searrow -1} \sup_{\substack{x \in [\frac{1}{2}(1 + a_-(\eta_3)), \frac{1}{2}(a_-(\eta_3) + a_+(\eta_3))] \\ \eta \in [\eta_4, \eta_3]}} |w(x, y, \eta) - \tilde{w}(x, -1, \eta)| = 0.$$

(ii): Take any  $s \in (0, \frac{1}{8}]$ . By (3.1), (3.2) there exists  $\hat{\eta}_3 \in (0, 17 - 12\sqrt{2})$  such that  $\tilde{w}(a_+(\hat{\eta}_3), -1, \hat{\eta}_3) = s$ . We can choose  $\eta_1 \in (\hat{\eta}_3, 17 - 12\sqrt{2})$ ,  $\eta_2 \in (0, \hat{\eta}_3)$  sufficiently close to  $\hat{\eta}_3$  so that the same inequalities as (3.5), (3.6), (3.7), (3.8) hold. Then by applying the uniform convergence property of the form (3.9) we obtain the claimed inequalities.  $\square$

*Proof of Proposition 3.1.* We set

$$s := \frac{b - b'}{b'}, \quad \eta := \left( \frac{e_{\min}}{e_{\max}} \right)^2$$

during the proof. First of all we note that

$$(3.10) \quad F_\infty(x, y) = D_d \int_{\Gamma_\infty^*} d\mathbf{k} \operatorname{Tr} \left( \frac{\sinh(xE_b(\mathbf{k}))}{(y + \cosh(xE_b(\mathbf{k})))E_b(\mathbf{k})} \right) = \frac{b'}{e_{\max}} W(e_{\max}x, y, \sqrt{\eta}, s),$$

which together with (2.61) implies that

$$(3.11) \quad \begin{aligned} \frac{\partial F_\infty}{\partial x}(\sqrt{y+1}x, y) &= b' \frac{1 + y \cosh(\sqrt{\eta(y+1)}e_{\max}x)}{(y + \cosh(\sqrt{\eta(y+1)}e_{\max}x))^2} \left( s - w \left( \frac{e_{\max}^2 x^2}{2}, y, \eta \right) \right), \\ \forall y \in (-1, 0), \quad x \in \left(0, \frac{\cosh^{-1}(|y|^{-1})}{e_{\min}\sqrt{y+1}}\right). \end{aligned}$$

We will also use the following convergence property.

$$(3.12) \quad \lim_{y \searrow -1} \sqrt{y+1} W(\sqrt{y+1}x, y, \sqrt{\xi}, s) = \widehat{W}(x, \sqrt{\xi}, s)$$

locally uniformly with  $(x, \xi) \in \mathbb{R}_{>0} \times \mathbb{R}_{>0}$ .

(i): Assume that  $s \in [3 - 2\sqrt{2}, \infty)$ . If  $\frac{e_{\min}}{e_{\max}} > \sqrt{17 - 12\sqrt{2}}$ , Proposition 2.11 ensures the result. Assume that  $\frac{e_{\min}}{e_{\max}} = \sqrt{17 - 12\sqrt{2}}$ . Here we apply [25, Lemma 2.24 (i)] to guarantee that

$$(3.13) \quad \begin{aligned} &\exists y_0 \in (-1, 0) \text{ s.t.} \\ &\forall y \in (-1, y_0] \exists x_0(y) \in \left( \frac{1}{2(y+1)}(\cosh^{-1}(|y|^{-1}))^2, \frac{1}{2\eta(y+1)}(\cosh^{-1}(|y|^{-1}))^2 \right) \text{ s.t.} \\ &w(x, y, \eta) < s, \quad \forall x \in \left( \frac{1}{2(y+1)}(\cosh^{-1}(|y|^{-1}))^2, x_0(y) \right), \\ &w(x_0(y), y, \eta) = s, \\ &w(x, y, \eta) > s, \quad \forall x \in \left( x_0(y), \frac{1}{2\eta(y+1)}(\cosh^{-1}(|y|^{-1}))^2 \right). \end{aligned}$$

Since

$$\frac{\partial F_\infty}{\partial x}(\sqrt{y+1}x, y) > 0, \quad \forall x \in \left( 0, \frac{\cosh^{-1}(|y|^{-1})}{e_{\max}\sqrt{y+1}} \right],$$

$$\frac{\partial F_\infty}{\partial x}(\sqrt{y+1}x, y) < 0, \quad \forall x \in \left[ \frac{\cosh^{-1}(|y|^{-1})}{e_{\min}\sqrt{y+1}}, \infty \right)$$

for any  $y \in (-1, 0)$ , combination of (3.11) and (3.13) proves that for any  $y \in (-1, y_0]$  there exists  $\hat{x}_0 \in (\frac{\cosh^{-1}(|y|^{-1})}{e_{\max}}, \frac{\cosh^{-1}(|y|^{-1})}{e_{\min}})$  such that

$$\begin{aligned} \frac{\partial F_\infty}{\partial x}(x, y) &> 0, \quad \forall x \in (0, \hat{x}_0), \\ \frac{\partial F_\infty}{\partial x}(\hat{x}_0, y) &= 0, \\ \frac{\partial F_\infty}{\partial x}(x, y) &< 0, \quad \forall x \in (\hat{x}_0, \infty). \end{aligned}$$

Now the assumption of Lemma 2.7 with  $S = \{E_b\}$  is satisfied and thus the claim follows from the lemma in this case.

Assume that  $\frac{e_{\min}}{e_{\max}} < \sqrt{17 - 12\sqrt{2}}$ . By (3.1) and (3.3)  $s \in (\tilde{w}(a_-(\eta), -1, \eta), \infty)$ . Thus we can apply [25, Lemma 2.24 (ii)] to ensure that the property (3.13) holds. Then by repeating the same argument as above and using Lemma 2.7 we can deduce the claim in this case as well. The proof of (i) is complete.

(ii): Assume that  $s \in (\frac{1}{8}, 3 - 2\sqrt{2})$ . Take any  $e_{\min} \in \mathbb{R}_{>0}$  and  $U_0 \in (0, \frac{2e_{\min}}{b})$ . Let  $\eta_1, \eta_2, \eta_3, \eta_4 \in (0, 17 - 12\sqrt{2})$ ,  $y_1 \in (-1, 0)$  be those introduced in Lemma 3.3 (i). We can see from (3.10) that for any

$$e_{\max} \in \left[ \frac{e_{\min}}{\sqrt{\eta_1}}, \frac{e_{\min}}{\sqrt{\eta_2}} \right], \quad x \in \left[ \frac{\sqrt{1 + a_-(\eta_2)}}{e_{\max}}, \frac{\sqrt{a_+(\eta_2) + \eta_1^{-1}}}{e_{\max}} \right], \quad y \in (-1, 0)$$

$$\begin{aligned} (3.14) \quad & \sqrt{y+1}F_\infty(\sqrt{y+1}x, y) \\ & \geq \frac{b'\sqrt{\eta_2}}{e_{\min}} \inf_{\substack{x \in [\sqrt{1+a_-(\eta_2)}, \sqrt{a_+(\eta_2)+\eta_1^{-1}}] \\ \xi \in [\eta_2, \eta_1]}} \sqrt{y+1}W(\sqrt{y+1}x, y, \sqrt{\xi}, s). \end{aligned}$$

By the convergence property (3.12) there exists  $y_2 \in (-1, y_1]$  such that for any  $y \in (-1, y_2]$

$$\begin{aligned} (3.15) \quad & \inf_{\substack{x \in [\sqrt{1+a_-(\eta_2)}, \sqrt{a_+(\eta_2)+\eta_1^{-1}}] \\ \xi \in [\eta_2, \eta_1]}} \sqrt{y+1}W(\sqrt{y+1}x, y, \sqrt{\xi}, s) \\ & \geq \frac{1}{2} \inf_{\substack{x \in [\sqrt{1+a_-(\eta_2)}, \sqrt{a_+(\eta_2)+\eta_1^{-1}}] \\ \xi \in [\eta_2, \eta_1]}} \widehat{W}(x, \sqrt{\xi}, s). \end{aligned}$$

We can derive from (2.46), (3.14), (3.15) that there exists  $\hat{y} \in (-1, y_2]$  such that

$$(3.16) \quad F_\infty(\sqrt{\hat{y}+1}x, \hat{y}) \geq \frac{2}{U_0}, \quad \forall e_{\max} \in \left[ \frac{e_{\min}}{\sqrt{\eta_1}}, \frac{e_{\min}}{\sqrt{\eta_2}} \right], \quad x \in \left[ \frac{\sqrt{1 + a_-(\eta_2)}}{e_{\max}}, \frac{\sqrt{a_+(\eta_2) + \eta_1^{-1}}}{e_{\max}} \right],$$

$$(3.17) \quad \frac{\cosh^{-1}(|\hat{y}|^{-1})}{\sqrt{\hat{y}+1}} > \sqrt{2}.$$

It follows from the inequalities claimed in Lemma 3.3 (i) that there exists  $\hat{\eta}_1 \in (\eta_2, \eta_1)$  such that

$$\min_{x \in [\frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), \frac{1}{2}(a_+(\eta_2) + \eta_1^{-1})]} w(x, \hat{y}, \hat{\eta}_1) = s,$$

$$w\left(\frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), \hat{y}, \hat{\eta}_1\right) > s, \quad w\left(\frac{1}{2}(a_+(\eta_2) + \eta_1^{-1}), \hat{y}, \hat{\eta}_1\right) > s.$$

Let  $x_0 \in (\frac{1}{2}(a_-(\eta_2) + a_+(\eta_2)), \frac{1}{2}(a_+(\eta_2) + \eta_1^{-1}))$  be a minimizer. Set

$$e_{max} := \frac{e_{min}}{\sqrt{\hat{\eta}_1}}, \quad \hat{x} := \frac{\sqrt{2(\hat{y} + 1)x_0}}{e_{max}}.$$

By (3.16)

$$(3.18) \quad F_\infty(\hat{x}, \hat{y}) \geq \frac{2}{U_0}.$$

Observe that by (3.17)

$$\frac{\sqrt{2x_0}}{e_{max}} < \frac{\sqrt{a_+(\eta_2) + \eta_1^{-1}}}{e_{max}} < \frac{\sqrt{2\eta_1^{-1}}}{e_{max}} < \frac{\sqrt{2\hat{\eta}_1^{-1}}}{e_{max}} = \frac{\sqrt{2}}{e_{min}} < \frac{\cosh^{-1}(|\hat{y}|^{-1})}{e_{min}\sqrt{\hat{y} + 1}},$$

and thus by (3.11)

$$(3.19) \quad \frac{\partial F_\infty}{\partial x}(\hat{x}, \hat{y}) = b' \frac{1 + \hat{y} \cosh(\sqrt{2\hat{\eta}_1(\hat{y} + 1)x_0})}{(\hat{y} + \cosh(\sqrt{2\hat{\eta}_1(\hat{y} + 1)x_0}))^2} (s - w(x_0, \hat{y}, \hat{\eta}_1)) = 0.$$

We remark that by (3.17)

$$\sqrt{2\hat{\eta}_1(\hat{y} + 1)x_0} < \sqrt{\hat{\eta}_1(\hat{y} + 1)(a_+(\eta_2) + \eta_1^{-1})} < \sqrt{2\hat{\eta}_1(\hat{y} + 1)\eta_1^{-1}} < \sqrt{2(\hat{y} + 1)}$$

$$< \cosh^{-1}(|\hat{y}|^{-1}),$$

and thus

$$1 + \hat{y} \cosh(\sqrt{2\hat{\eta}_1(\hat{y} + 1)x_0}) > 0.$$

We can deduce from this inequality and the definition of  $x_0$  that there exists  $\varepsilon \in \mathbb{R}_{>0}$  such that  $\frac{\partial F_\infty}{\partial x}(x, \hat{y}) < 0$  for any  $x \in (\hat{x} - \varepsilon, \hat{x} + \varepsilon) \setminus \{\hat{x}\}$ . This together with (3.18), (3.19) enables us to apply Lemma 2.8 (ii) to conclude that there exists  $U \in [-U_0, 0)$  such that  $\tau(\cdot)$  has a rising SPI in  $(0, \beta_c)$ . Remind us that  $\frac{e_{min}}{e_{max}} = \sqrt{\hat{\eta}_1} \in (\sqrt{\eta_2}, \sqrt{\eta_1})$ . The existence of a rising SPI is now proved with  $e_1 = \sqrt{\hat{\eta}_1}$ .

The existence of a falling SPI can be proved similarly. However, we provide the proof for completeness. We can derive from (3.10) that for any

$$e_{max} \in \left[ \frac{e_{min}}{\sqrt{\eta_3}}, \frac{e_{min}}{\sqrt{\eta_4}} \right], \quad x \in \left[ \frac{\sqrt{1 + a_-(\eta_3)}}{e_{max}}, \frac{\sqrt{a_-(\eta_3) + a_+(\eta_3)}}{e_{max}} \right], \quad y \in (-1, 0)$$

$$\sqrt{y + 1}F_\infty(\sqrt{y + 1}x, y)$$

$$\geq \frac{b' \sqrt{\eta_4}}{e_{min}} \inf_{\substack{x \in [\sqrt{1 + a_-(\eta_3)}, \sqrt{a_-(\eta_3) + a_+(\eta_3)}] \\ \xi \in [\eta_4, \eta_3]}} \sqrt{y + 1}W(\sqrt{y + 1}x, y, \sqrt{\xi}, s).$$

Application of (3.12) yields that there exists  $y_3 \in (-1, y_1]$  such that for any  $y \in (-1, y_3]$

$$\begin{aligned} & \inf_{\substack{x \in [\sqrt{1+a_-(\eta_3)}, \sqrt{a_-(\eta_3)+a_+(\eta_3)}] \\ \xi \in [\eta_4, \eta_3]}} \sqrt{y+1} W(\sqrt{y+1}x, y, \sqrt{\xi}, s) \\ & \geq \frac{1}{2} \inf_{\substack{x \in [\sqrt{1+a_-(\eta_3)}, \sqrt{a_-(\eta_3)+a_+(\eta_3)}] \\ \xi \in [\eta_4, \eta_3]}} \widehat{W}(x, \sqrt{\xi}, s). \end{aligned}$$

We can deduce from these inequalities and (2.46) that there exists  $\tilde{y} \in (-1, y_3]$  such that

$$\begin{aligned} (3.20) \quad & F_\infty(\sqrt{\tilde{y}+1}x, \tilde{y}) \geq \frac{2}{U_0}, \quad \forall e_{max} \in \left[ \frac{e_{min}}{\sqrt{\eta_3}}, \frac{e_{min}}{\sqrt{\eta_4}} \right], \quad x \in \left[ \frac{\sqrt{1+a_-(\eta_3)}}{e_{max}}, \frac{\sqrt{a_-(\eta_3)+a_+(\eta_3)}}{e_{max}} \right], \\ (3.21) \quad & \frac{\cosh^{-1}(|\tilde{y}|^{-1})}{\sqrt{\tilde{y}+1}} > \sqrt{2}. \end{aligned}$$

The inequalities of Lemma 3.3 (i) imply that there exists  $\hat{\eta}_2 \in (\eta_4, \eta_3)$  such that

$$\begin{aligned} & \max_{x \in [\frac{1}{2}(1+a_-(\eta_3)), \frac{1}{2}(a_-(\eta_3)+a_+(\eta_3))]} w(x, \tilde{y}, \hat{\eta}_2) = s, \\ & w\left(\frac{1}{2}(1+a_-(\eta_3)), \tilde{y}, \hat{\eta}_2\right) < s, \quad w\left(\frac{1}{2}(a_-(\eta_3)+a_+(\eta_3)), \tilde{y}, \hat{\eta}_2\right) < s. \end{aligned}$$

Let  $\tilde{x}_0 \in (\frac{1}{2}(1+a_-(\eta_3)), \frac{1}{2}(a_-(\eta_3)+a_+(\eta_3)))$  be a maximizer and set

$$e_{max} := \frac{e_{min}}{\sqrt{\hat{\eta}_2}}, \quad \tilde{x} := \frac{\sqrt{2(\tilde{y}+1)\tilde{x}_0}}{e_{max}}.$$

By (3.20)

$$(3.22) \quad F_\infty(\tilde{x}, \tilde{y}) \geq \frac{2}{U_0}.$$

Moreover, by (3.21)

$$\frac{\sqrt{2\tilde{x}_0}}{e_{max}} < \frac{\sqrt{a_-(\eta_3)+a_+(\eta_3)}}{e_{max}} < \frac{\sqrt{2\eta_3^{-1}}}{e_{max}} < \frac{\sqrt{2\hat{\eta}_2^{-1}}}{e_{max}} = \frac{\sqrt{2}}{e_{min}} < \frac{\cosh^{-1}(|\tilde{y}|^{-1})}{e_{min}\sqrt{\tilde{y}+1}},$$

and thus by (3.11)

$$(3.23) \quad \frac{\partial F_\infty}{\partial x}(\tilde{x}, \tilde{y}) = b' \frac{1 + \tilde{y} \cosh(\sqrt{2\hat{\eta}_2(\tilde{y}+1)\tilde{x}_0})}{(\tilde{y} + \cosh(\sqrt{2\hat{\eta}_2(\tilde{y}+1)\tilde{x}_0}))^2} (s - w(\tilde{x}_0, \tilde{y}, \hat{\eta}_2)) = 0.$$

By using (3.21) again we can derive that

$$\begin{aligned} \sqrt{2\hat{\eta}_2(\tilde{y}+1)\tilde{x}_0} & < \sqrt{\hat{\eta}_2(\tilde{y}+1)(a_-(\eta_3)+a_+(\eta_3))} < \sqrt{2\hat{\eta}_2(\tilde{y}+1)\eta_3^{-1}} < \sqrt{2(\tilde{y}+1)} \\ & < \cosh^{-1}(|\tilde{y}|^{-1}), \end{aligned}$$

and thus

$$1 + \tilde{y} \cosh(\sqrt{2\hat{\eta}_2(\tilde{y} + 1)\tilde{x}_0}) > 0.$$

By considering this inequality we can deduce from (3.23) and the definition of  $\tilde{x}_0$  that there exists  $\tilde{\varepsilon} \in \mathbb{R}_{>0}$  such that  $\frac{\partial F_\infty}{\partial x}(x, \tilde{y}) > 0$  for any  $x \in (\tilde{x} - \tilde{\varepsilon}, \tilde{x} + \tilde{\varepsilon}) \setminus \{\tilde{x}\}$ . This coupled with (3.23) means that  $\tilde{x}$  is a rising SPI of  $F_\infty(\cdot, \tilde{y})$ . Since we have (3.22), we can apply Lemma 2.8 (i) to ensure that there exists  $U \in [-U_0, 0)$  such that  $\tau(\cdot)$  has a falling SPI in  $(0, \beta_c)$ . Here  $\frac{e_{\min}}{e_{\max}} = \sqrt{\hat{\eta}_2} \in (\sqrt{\eta_4}, \sqrt{\eta_3})$ .

Now we can see that the claim (ii) holds with  $e_1 = \sqrt{\hat{\eta}_1}$ ,  $e_2 = \sqrt{\hat{\eta}_2}$ .

(iii): By using Lemma 3.3 (ii) in place of Lemma 3.3 (i) we can repeat the same argument as the 1st half of the proof of (ii) to prove the claim.  $\square$

In [25, Proposition 2.25] we derived  $\tau(\beta)$  exactly. Let us numerically implement the exact solution to observe that  $\tau(\cdot)$  has SPIs as suggested by Proposition 3.1. We set  $b = 8$ ,  $b' = 7$ ,  $e_{\min} = 1$ ,  $U = -\frac{1}{8}$  so that  $\frac{b-b'}{b'} \in (\frac{1}{8}, 3-2\sqrt{2})$ ,  $|U| \in (0, \frac{2e_{\min}}{b})$ . In fact these parameters take the same values as in the numerical example in [25, Sub-subsection 2.3.1]. Based on Proposition 3.1 (ii), we expect that we can find  $e_1, e_2 \in (0, \sqrt{17-12\sqrt{2}})$  such that  $e_2 < e_1$  and if  $e_{\max} = \frac{1}{e_1}$ ,  $\tau(\cdot)$  has a rising SPI, if  $e_{\max} = \frac{1}{e_2}$ ,  $\tau(\cdot)$  has a falling SPI. In Figure 4 we plot the graphs of  $\tau(\beta)$ ,  $\frac{d\tau}{d\beta}(\beta)$  for  $e_{\max} = 6.643, 8.342$ . We can see that  $\tau(\cdot)$  has a rising SPI when  $e_{\max} = 6.643$  and  $\tau(\cdot)$  has a falling SPI when  $e_{\max} = 8.342$ . This means that our expectation is realized with  $e_1 = \frac{1}{6.643} (\approx 0.1505)$ ,  $e_2 = \frac{1}{8.342} (\approx 0.1199) \in (0, \sqrt{17-12\sqrt{2}}) (\approx (0, 0.1716))$ .

Concerning the model (2), we claim the following proposition. In fact it is an immediate consequence of Lemma 2.7 and the proof of [25, Proposition 2.26].

**Proposition 3.5.** *For any  $t \in \mathbb{R}_{\geq 0}$ ,  $e_{\min} \in \mathbb{R}_{>0}$  there exists  $U_0 \in (0, 2e_{\min})$  such that for any  $U \in [-U_0, 0)$   $\tau(\cdot)$  has no SPI in  $(0, \beta_c)$ .*

*Proof.* We have shown in the proof of [25, Proposition 2.26] that there exists  $y_0 \in (-1, 0)$  such that for any  $y \in (-1, y_0]$  there uniquely exists  $x_0 \in \mathbb{R}_{>0}$  such that  $\frac{\partial F_\infty}{\partial x}(x_0, y) = 0$ . See around the equation “(2.101)” in [25]. Then Lemma 2.7 with  $S = \{E_1\}$  ensures the result.  $\square$

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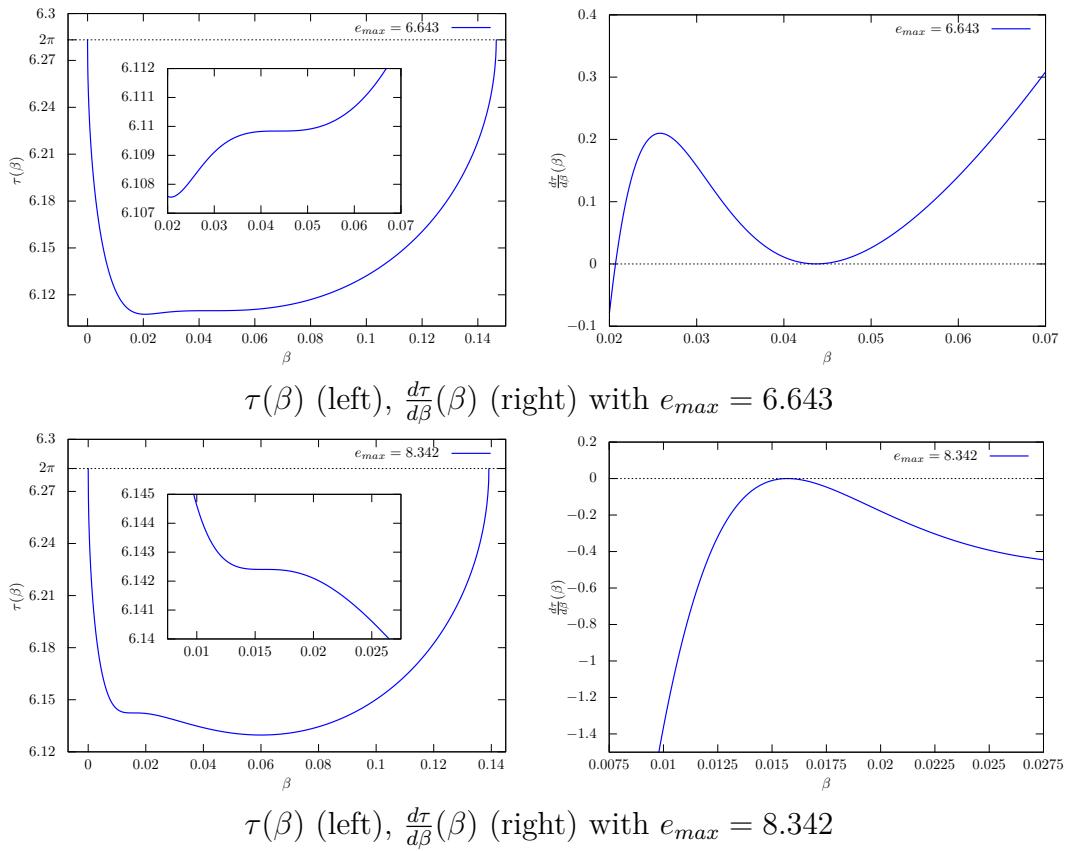


Figure 4: Parts of the graphs  $\{(\beta, \tau(\beta)) \mid \beta \in (0, \beta_c)\}$ ,  $\{(\beta, \frac{d\tau}{d\beta}(\beta)) \mid \beta \in (0, \beta_c)\}$  for  $b = 8$ ,  $b' = 7$ ,  $U = -\frac{1}{8}$ ,  $e_{min} = 1$ ,  $e_{max} = 6.643, 8.342$ . The exact solution was implemented.

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