Analysis of phase transitions in the BCS model with imaginary magnetic field

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1 Introduction

This article is essentially a summary of the author's talk given in 10:00–10:50, December 6th, 2021 as part of the online workshop "Mathematical Aspects of Quantum Fields and Related Topics". We are going to present mathematical propositions and theorems explained in the talk. However, we do not provide any proof for the claims here. Instead, we provide clear citations so that the readers can find the proofs in the original research papers [4], [5], [6], [7], mostly in [6], [7]. The author hopes that this article helps the readers recall his talk and could be an introduction to [4], [5], [6], [7].

2 The BCS model with imaginary magnetic field

Let us begin by defining the BCS model with imaginary magnetic field. Let b, d, $L \in \mathbb{N}$. Let $\{\mathbf{v}_j\}_{j=1}^{d}$ be a basis of $\mathbb{R}^d$ and $\{\hat{\mathbf{v}}_j\}_{j=1}^{d}$ be its dual basis. The spatial lattice Γ and the momentum lattice Γ^* are defined by

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

$$\Gamma^* := \left\{ \sum_{j=1}^{d} \hat{m}_j \hat{\mathbf{v}}_j \ \middle| \ \hat{m}_j \in \left\{0, \frac{2\pi}{L}, \frac{4\pi}{L}, \cdots, 2\pi - \frac{2\pi}{L}\right\} \ (j = 1, \cdots, d) \right\}.$$

In fact we consider a more general spatial lattice which has b sites in its unit cell. Set $\mathcal{B} := \{1, \cdots, b\}$. The generalized spatial lattice is identified as $\mathcal{B} \times \Gamma$. Here we assume that the one-particle free Hamiltonian E satisfies the following conditions with momentum variables.

$$\begin{aligned}
&E \in C^\infty(\mathbb{R}^d, \mathrm{Mat}(b, \mathbb{C})),\\
&E(\mathbf{k}) = E(\mathbf{k})^*,\\
&E(\mathbf{k} + 2\pi \hat{\mathbf{v}}_j) = E(\mathbf{k}),\\
&E(\mathbf{k}) = \overline{E(-\mathbf{k})}, \ \forall \mathbf{k} \in \mathbb{R}^d, \ j \in \{1, \cdots, d\}.
\end{aligned}$$

The free Hamiltonian H_0, the BCS interaction V, the BCS model H are defined as operators on the Fermionic Fock space $F_f(L^2(\mathcal{B}\times\Gamma\times\{\uparrow,\downarrow\}))$.

$$\begin{aligned}
H_0 &:= \frac{1}{L^d}\sum_{(\rho,\mathbf{x}),(\eta,\mathbf{y})\in\mathcal{B}\times\Gamma}\sum_{\sigma\in\{\uparrow,\downarrow\}}\sum_{\mathbf{k}\in\Gamma^*} e^{i\langle\mathbf{x}-\mathbf{y},\mathbf{k}\rangle}E(\mathbf{k})(\rho,\eta)\psi^*_{\rho\mathbf{x}\sigma}\psi_{\eta\mathbf{y}\sigma},\\
V &:= \frac{U}{L^d}\sum_{(\rho,\mathbf{x}),(\eta,\mathbf{y})\in\mathcal{B}\times\Gamma}\psi^*_{\rho\mathbf{x}\uparrow}\psi^*_{\rho\mathbf{x}\downarrow}\psi_{\eta\mathbf{y}\downarrow}\psi_{\eta\mathbf{y}\uparrow},\ U<0,\\
H &:= H_0+V.
\end{aligned}$$

The parameter $U(\in\mathbb{R}_{<0})$ controls the strength of attractive interaction between Cooper pairs. Because of the simplicity that the spatial variables $\mathbf{x}$, $\mathbf{y}$ move independently, V is sometimes called the reduced BCS interaction. Since it has the reduced interaction, H is sometimes called the reduced BCS model. The main novelty of the series [4], [5], [6] is that the interaction with imaginary magnetic field is modeled by adding the operator itS_z to the Hamiltonian, where $t\in\mathbb{R}$ and S_z is the z-component of spin operator defined by

$$S_z := \frac{1}{2}\sum_{(\rho,\mathbf{x})\in\mathcal{B}\times\Gamma}(\psi^*_{\rho\mathbf{x}\uparrow}\psi_{\rho\mathbf{x}\uparrow}-\psi^*_{\rho\mathbf{x}\downarrow}\psi_{\rho\mathbf{x}\downarrow}).$$

The operator $H+itS_z$ is non-hermitian, which makes well-definedness of thermodynamic quantities such as free energy density or thermal expectation values non-trivial. We explicitly derived their infinite-volume limit in [4], [5], [6]. For instance the infinite-volume limit of the 4-point correlation function

$$\lim_{\substack{L\to\infty\\ L\in\mathbb{N}}}\frac{\mathrm{Tr}(e^{-\beta H+itS_z}\psi^*_{\rho\mathbf{x}\uparrow}\psi^*_{\rho\mathbf{x}\downarrow}\psi_{\eta\mathbf{y}\downarrow}\psi_{\eta\mathbf{y}\uparrow})}{\mathrm{Tr}\, e^{-\beta H+itS_z}}$$

was derived and proved to show off-diagonal long range order, which is a characteristic of superconducting order. Let us explain the applicability of the main theorems when the free dispersion relation is that of nearest-neighbor hopping electron, namely

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

- [4, Theorem 1.3] applies to the case where $d\in\mathbb{N}$ and $|\mu|<2d$.
- [5, Theorem 1.3] applies to the case where $d\in\{3,4\}$ and $|\mu|=2d$.
- [6, Theorem 1.3] applies to the case where $d\in\mathbb{N}$ and $|\mu|>2d$.

In [6] we introduced a set of one-particle Hamiltonians $\mathcal{E}(e_{min},e_{max})$ $(0<e_{min}\le e_{max})$ as follows. $E\in\mathcal{E}(e_{min},e_{max})$ if and only if

$$\begin{aligned}
&E\in C^\infty(\mathbb{R}^d,\mathrm{Mat}(b,\mathbb{C})),\\
&E(\mathbf{k})=E(\mathbf{k})^*,\\
&E(\mathbf{k}+2\pi\hat{\mathbf{v}}_j)=E(\mathbf{k}),
\end{aligned}$$

$$
\begin{aligned}
&E(\mathbf{k}) = \overline{E(-\mathbf{k})},\ \forall \mathbf{k} \in \mathbb{R}^d,\ j \in \{1, \cdots, d\},\\
&\inf_{\mathbf{k}\in\mathbb{R}^d} \inf_{\substack{\mathbf{u}\in\mathbb{C}^b \\ \text{with } \|\mathbf{u}\|_{\mathbb{C}^b}=1}} \|E(\mathbf{k})\mathbf{u}\|_{\mathbb{C}^b} = e_{min},\\
&\sup_{\mathbf{k}\in\mathbb{R}^d} \|E(\mathbf{k})\|_{b\times b} = e_{max},
\end{aligned}
$$

where $\|\cdot\|_{\mathbb{C}^b}$ is the canonical norm of $\mathbb{C}^b$ and $\|\cdot\|_{b\times b}$ is the operator norm of $\mathrm{Mat}(b, \mathbb{C})$.

Fix $E \in \mathcal{E}(e_{min}, e_{max})$ and $U \in \mathbb{R}_{<0}$ sufficiently close to 0. Within the framework of [6] we can derive the infinite-volume limit of thermodynamic quantities for any inverse temperature $\beta(\in \mathbb{R}_{>0})$ and imaginary magnetic field $t(\in \mathbb{R})$. Phase transitions are proved to occur. Moreover, the phase diagram is fully drawn in the 2D plane of (inverse temperature, imaginary magnetic field). This means that we have more freedom to analyze the phase transition driven by temperature and imaginary magnetic field than in [4], [5] where the range of these parameters are restricted. For this reason we wish to focus on the situation of [6]. Our aim is to analyze the free energy density derived in [6].

Theorem 2.1 ([6, Theorem 1.3])**.** *There exists $c' \in (0, 1]$ depending only on d, b, $(\hat{\mathbf{v}}_j)_{j=1}^d$ and the quantity*

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

such that for any $U \in (-\frac{2c'}{b}\min\{e_{min}, e_{min}^{d+1}\}, 0)$, $\beta \in \mathbb{R}_{>0}$, $t \in \mathbb{R}$

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

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

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

and $\Delta \in \mathbb{R}_{\ge 0}$ is defined as follows. $\Delta := 0$ if

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

Otherwise, $\Delta \ge 0$ is the unique solution to

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

The singularity of the function

$$t \mapsto \lim_{\substack{L\to\infty \\ L\in\mathbb{N}}} \left(-\frac{1}{\beta L^d} \log(\mathrm{Tr}\, e^{-\beta H + itS_z}) \right)$$

indicates existence of dynamical phase transition at positive temperature. To the author's knowledge, the concept was first introduced in [1], [3], though the zero temperature version goes back earlier. In this context "t" is considered as the real time variable.

To set up our goals, let us explicitly define the free energy density as a function of $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$. First we need to make clear the well-posedness of our gap equation. For $E \in \mathcal{E}(e_{min}, e_{max})$, define the function $g_E : \mathbb{R}_{>0} \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ by

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

Our gap equation is to find $\Delta \in \mathbb{R}_{\geq 0}$ such that $g_E(\beta, t, \Delta) = 0$. The next lemma characterizes unique solvability of the gap equation.

Lemma 2.2 ([6, Lemma 1.1])**.** *Let* $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$. *There uniquely exists* $\Delta \in \mathbb{R}_{\geq 0}$ *such that* $g_E(\beta, t, \Delta) = 0$ *if and only if* $g_E(\beta, t, 0) \geq 0$.

Based on the above lemma, we can define the gap function $\Delta : \mathbb{R}_{>0} \times \mathbb{R} \to \mathbb{R}_{\geq 0}$ as follows. If $g_E(\beta, t, 0) \geq 0$, $\Delta(\beta, t)$ is the solution to $g_E(\beta, t, \Delta) = 0$. If $g_E(\beta, t, 0) < 0$, set $\Delta(\beta, t) := 0$. Substitution of the gap function enables us to define the free energy density as a function of $(\beta, t) \in \mathbb{R}_{>0} \times \mathbb{R}$.

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

After these preparations we can summarize what we want to achieve.

- Characterize the boundary of the set of (β, t) ($\subset \mathbb{R}_{>0} \times \mathbb{R}$) where $\Delta(\beta, t) > 0$. In other words this is to analyze the phase boundary.
- Characterize the regularity of $(\beta, t) \mapsto F_E(\beta, t)$. By analogy with the Ehrenfest classification this is to analyze the order of phase transition.

We will explain these projects in the rest of this article.

3 Analysis of the phase boundary

Define the subset Q_+, Q_-, Q_0 of $\mathbb{R}_{>0} \times \mathbb{R}$ by

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

$$Q_0 := \{(\beta,t)\in\mathbb{R}_{>0}\times\mathbb{R} \mid g_E(\beta,t,0)=0\}.$$

One can see that

$$\mathbb{R}_{>0}\times\mathbb{R} = Q_+ \sqcup Q_- \sqcup Q_0,\ Q_+ = \{(\beta,t)\in\mathbb{R}_{>0}\times\mathbb{R} \mid \Delta(\beta,t)>0\}.$$

Let us call Q_0 phase boundary. We must confirm that the phase boundary is non-empty. The next lemma not only answers this question but ensures that the critical inverse temperature exists as a terminal point of the phase boundary.

Lemma 3.1 ([6, Lemma 1.2, Lemma 2.2])**.** *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 the following statements hold.*

- $g_E(\beta,t,0)<0,\ \forall\beta\in(\beta_c,\infty),\ t\in\mathbb{R}.$
- $\sup_{t\in\mathbb{R}} g_E(\beta_c,t,0) = g_E(\beta_c,2\pi,0)=0.$
- $\forall\beta\in(0,\beta_c)\ \exists!\tau(\beta)\in(\pi,2\pi)\ s.t.\ g_E(\beta,\tau(\beta),0)=0.$

Moreover, $\tau\in C^\omega((0,\beta_c))$*,* $\lim_{\beta\nearrow\beta_c}\tau(\beta)=\lim_{\beta\searrow 0}\tau(\beta)=2\pi$*.*

From here we always assume $|U| < \frac{2e_{min}}{b}$ so that we can apply the above lemma. We can characterize Q_0 by parity and periodicity as follows.

Lemma 3.2 ([6, (2.3)])**.**

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

The lemma implies that Q_0 is a union of copies of

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

Based on this fact, we can sketch the phase diagram as in Figure 1. In view of the conventional physics of the BCS theory, it is counter-intuitive that the gap function $\Delta(\beta,t)$ can be positive only in high temperature.

Remark 3.3. Not to mislead the readers, we remark that our notion of phase diagram is different from the dynamical phase diagrams defined in the physics literature (e.g. [10], [2], [8], [9]). Our phase diagram corresponds to the boundary of a set of (inverse temperature, real time) where the gap equation has a positive solution. On the other hand, the dynamical phase diagrams in [10], [2], [8], [9] correspond to the boundary of a set of 2 parameters which do not include the real time variable. The 2 parameters plus the real time variable control a dynamical analogue of free energy density called return rate function. The 2 parameters belong to the set if the return rate function shows a particular singularity with respect to the time variable while these 2 parameters are fixed.

To analyze the phase boundary, it suffices to focus on the representative curve $\hat{Q}_0$ defined by

$$\hat{Q}_0 := \{(\beta,\tau(\beta)),\ (\beta,-\tau(\beta)+4\pi)\mid\beta\in(0,\beta_c)\}\cup\{(0,2\pi),\ (\beta_c,2\pi)\}.$$

This curve is in fact a nice mathematical object.

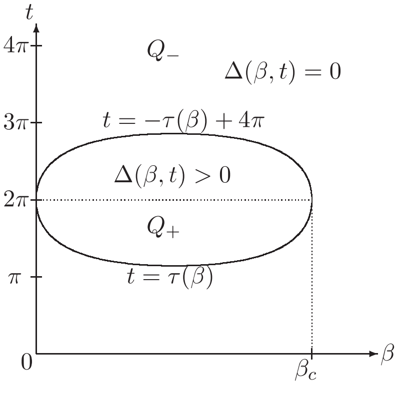


Figure 1: The schematic phase diagram

Proposition 3.4 ([6, Proposition 2.4]). *$\hat{Q}_0$ is a 1-dimensional real analytic submanifold of $\mathbb{R}^2$.*

However, the graph $\{(\beta,\tau(\beta)) \mid \beta \in (0,\beta_c)\}$ behaves in various ways.

Example 3.5 ([6, Proposition 2.25]). Consider the one-particle Hamiltonian E ($\in \mathcal{E}(e_{min}, e_{max})$) of non-hopping electron defined by

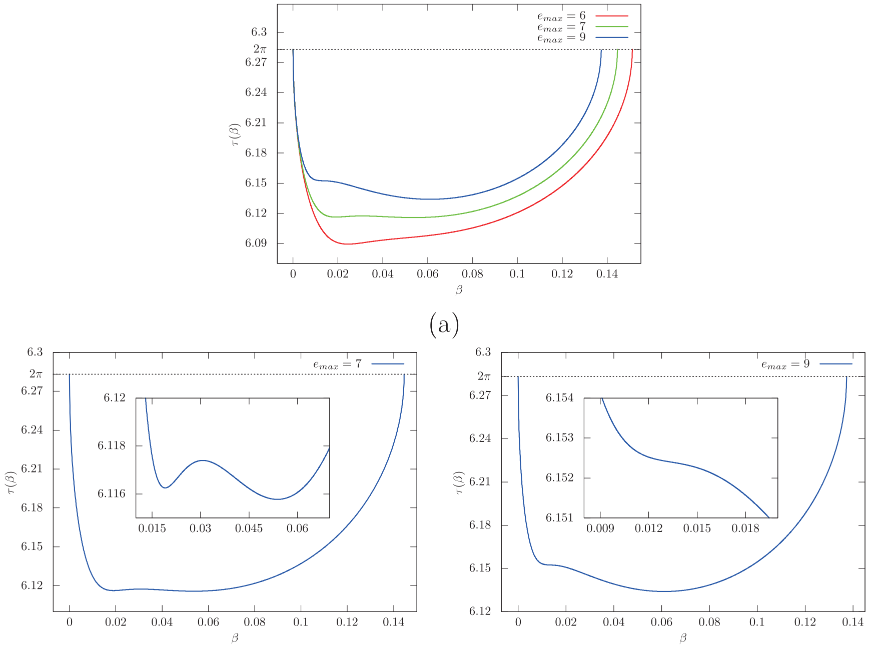
$$E(\mathbf{k}) = \begin{pmatrix} e_{max} I_{b'} & 0 \\ 0 & e_{min} I_{b-b'} \end{pmatrix},\ b \geq 2,\ b' \in \{1,2,\cdots,b-1\},$$

where I_n is the $n \times n$ unit matrix for $n \in \mathbb{N}$. In this case $\tau(\beta)$ ($\beta \in (0,\beta_c)$) is exactly obtained as below.

$$\begin{aligned}
&\tau(\beta) = 2\arccos\Big(\frac{-D_1 + \sqrt{D_1^2 - 4D_0}}{2}\Big),\\
&D_0 := \cosh(\beta e_{max})\cosh(\beta e_{min})\\
&\qquad - \frac{|U|}{2}\left(\frac{b'}{e_{max}}\sinh(\beta e_{max})\cosh(\beta e_{min}) + \frac{b-b'}{e_{min}}\cosh(\beta e_{max})\sinh(\beta e_{min})\right),\\
&D_1 := \cosh(\beta e_{max}) + \cosh(\beta e_{min}) - \frac{|U|}{2}\left(\frac{b'}{e_{max}}\sinh(\beta e_{max}) + \frac{b-b'}{e_{min}}\sinh(\beta e_{min})\right),
\end{aligned}$$

where $\arccos : [-1,1] \to [0,\pi]$ is the inverse function of $\cos|_{[0,\pi]}$. For example let $b = 8$, $b' = 7$, $U = -\frac{1}{8}$, $e_{min} = 1$. Then for $e_{max} = 6, 7, 9$ we can visualize the graph $\{(\beta,\tau(\beta)) \mid \beta \in (0,\beta_c)\}$ by implementing the exact solution in our PC. From (a) we can see that $\tau(\cdot)$ with $e_{max} = 6$ has only one local minimum point. By zooming separately in (b) we can see that $\tau(\cdot)$ with $e_{max} = 7$ has two local minimum points. Picture (c) shows that $\tau(\cdot)$ has only one local minimum point when $e_{max} = 9$.

The observation in the above example leads to the following question. What is a condition for $\tau(\cdot)$ to have only one local minimum point. The following theorem answers this question.



(a) (b) (c)

Theorem 3.6 ([6, Theorem 2.19]). *The following statements are equivalent to each other.*

(i) There exists $U_0 \in (0, \frac{2e_{min}}{b})$ *such that* $\tau(\cdot)$ *has only one local minimum point for any* $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$.

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

4 Analysis of the phase transition

According to the Ehrenfest classification, the order of phase transition is defined by regularity of the free energy. So let us study the regularity of the function $(\beta, t) \mapsto F_E(\beta, t)$. It is relatively straightforward to confirm the following.

Proposition 4.1 ([6, Proposition 2.5 (i)]).

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

However, the free energy density F_E is not smooth on the phase boundary Q_0. More detailed analysis reveals jump discontinuity of F_E on Q_0 as follows.

Proposition 4.2 ([6, Proposition 2.5 (ii), (iii)]).

(i) For any $(\beta_0, t_0) \in Q_0$, $\lim_{(\beta,t)\to(\beta_0,t_0),(\beta,t)\in Q_+} \frac{\partial^2 F_E}{\partial t^2}(\beta, t)$, $\lim_{(\beta,t)\to(\beta_0,t_0),(\beta,t)\in Q_-} \frac{\partial^2 F_E}{\partial t^2}(\beta, t)$ *converge to finite values. Moreover, for any* $\beta_0 \in (0, \beta_c)$

$$\lim_{\substack{t\to t_0\\(\beta_0,t)\in Q_+}} \frac{\partial^2 F_E}{\partial t^2}(\beta_0, t) < \lim_{\substack{t\to t_0\\(\beta_0,t)\in Q_-}} \frac{\partial^2 F_E}{\partial t^2}(\beta_0, t).$$

(ii) For any $(\beta_0, t_0) \in Q_0$, $\lim_{(\beta,t)\to(\beta_0,t_0),(\beta,t)\in Q_+} \frac{\partial^2 F_E}{\partial \beta^2}(\beta, t)$, $\lim_{(\beta,t)\to(\beta_0,t_0),(\beta,t)\in Q_-} \frac{\partial^2 F_E}{\partial \beta^2}(\beta, t)$ *converge to finite values. Moreover, for any* $\beta_0 \in (0, \beta_c)$ *with* $\frac{d\tau}{d\beta}(\beta_0) \neq 0$

$$\lim_{\substack{\beta\to \beta_0\\(\beta,t_0)\in Q_+}} \frac{\partial^2 F_E}{\partial \beta^2}(\beta, t_0) < \lim_{\substack{\beta\to \beta_0\\(\beta,t_0)\in Q_-}} \frac{\partial^2 F_E}{\partial \beta^2}(\beta, t_0).$$

(iii) For any $\beta_0 \in (0, \beta_c)$ *with* $\frac{d\tau}{d\beta}(\beta_0) = 0$

$$\lim_{\substack{\beta\to \beta_0\\(\beta,t_0)\in Q_+}} \frac{\partial^2 F_E}{\partial \beta^2}(\beta, t_0) = \lim_{\substack{\beta\to \beta_0\\(\beta,t_0)\in Q_-}} \frac{\partial^2 F_E}{\partial \beta^2}(\beta, t_0).$$

By analogy with the Ehrenfest classification the phase transition driven by t is of 2nd order. The phase transition driven by β is of 2nd order on most of the boundary points. According to (iii) of the above proposition, it may be higher order on a stationary point of the phase boundary. So we have the following question. How is a higher order phase transition (HOPT) driven by β related to a stationary point of inflection (SPI) of the phase boundary ? To answer this question systematically, we have to prepare several notions. First we classify the phase boundary Q_0 into the subsets $Q_{+,-}$, $Q_{-,+}$ defined by

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

for $(\rho, \eta) = (+, -)$, $(-, +)$. For any point of $Q_{\rho,\eta}$ there is a horizontal line passing through the point from Q_ρ to Q_η. We will study jump discontinuity of the derivatives of F_E along such a line. The curve Q_0 consists of $Q_{+,-}$, $Q_{-,+}$ plus local minimum/maximum points as sketched in Figure 2.

For $(\beta_0, t_0) \in \mathbb{R}_{>0} \times \mathbb{R}$, $n \in \mathbb{N}$, $(\rho, \eta) \in \{(+, -), (-, +)\}$ we define the conditions $(\mathrm{PT})_{n,(\rho,\eta)}(\beta_0, t_0)$, $(\mathrm{PT})_{n,(\rho,\eta)}$ by

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

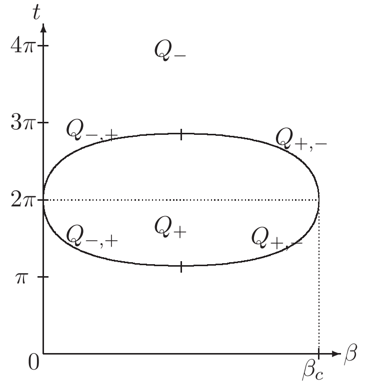


Figure 2: A classification of subsets of Q_0.

$$\begin{aligned}&(\mathrm{PT})_{n,(\rho,\eta)}: \\ &\quad \exists(\beta_0, t_0) \in \mathbb{R}_{>0} \times \mathbb{R} \text{ s.t. } (\mathrm{PT})_{n,(\rho,\eta)}(\beta_0, t_0) \text{ holds.}\end{aligned}$$

Moreover, we need to recall the definition of SPI.

Definition 4.3. Let $a, b, c \in \mathbb{R}$ satisfy $a < c < b$. Let $f \in C^1((a, b), \mathbb{R})$.

- We call c rising SPI if there exists $\varepsilon > 0$ such that $(c - \varepsilon, c + \varepsilon) \subset (a, b)$, $\frac{df}{dx}(c) = 0$, $\frac{df}{dx}(x) > 0$, $\forall x \in (c - \varepsilon, c + \varepsilon)\backslash\{c\}$.
- We call c falling SPI if there exists $\varepsilon > 0$ such that $(c - \varepsilon, c + \varepsilon) \subset (a, b)$, $\frac{df}{dx}(c) = 0$, $\frac{df}{dx}(x) < 0$, $\forall x \in (c - \varepsilon, c + \varepsilon)\backslash\{c\}$.

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

$$\begin{aligned}&(\mathrm{SPI})_r(\beta_0): \ \beta_0 \text{ is a rising SPI of } \tau(\cdot) : (0, \beta_c) \to \mathbb{R}. \\ &(\mathrm{SPI})_f(\beta_0): \ \beta_0 \text{ is a falling SPI of } \tau(\cdot) : (0, \beta_c) \to \mathbb{R}. \\ &(\mathrm{SPI})_\xi: \ \exists\beta_0 \in (0, \beta_c) \text{ s.t. } (\mathrm{SPI})_\xi(\beta_0) \text{ holds.}\end{aligned}$$

The relation between HOPT and SPI can be organized in terms of these notions.

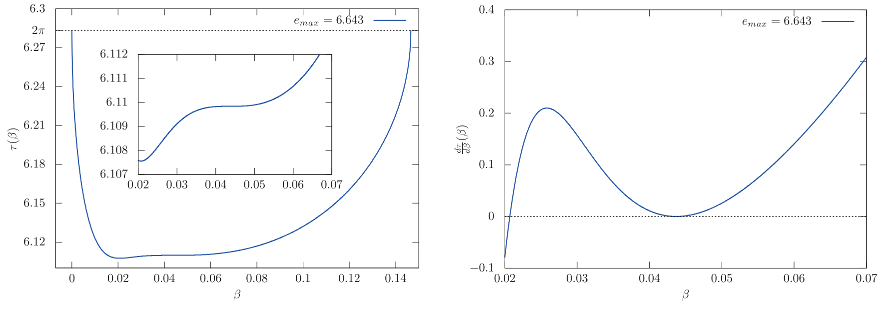
Theorem 4.4 ([7, Theorem 1.5])**.** *Let* $(\xi, \rho, \eta) \in \{(r, +, -), (f, -, +)\}$ *and* $\beta_0 \in (0, \beta_c)$.

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

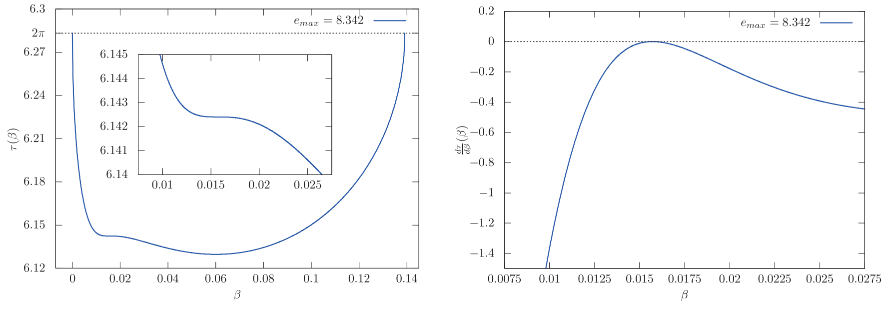
(ii) $(SPI)_\xi$ *does not hold if and only if* $(PT)_{2,(\rho,\eta)}(\beta, t)$ *holds for any* $(\beta, t) \in Q_{\rho,\eta}$.

(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.*

The above theorem itself does not imply existence of HOPT or equivalently SPI. The next theorem not only implies the existence but also provides a necessary and sufficient condition for the existence in terms of $\frac{e_{min}}{e_{max}}$.



$\tau(\beta)$ (left), $\frac{d\tau}{d\beta}(\beta)$ (right) with $e_{max} = 6.643$.



$\tau(\beta)$ (left), $\frac{d\tau}{d\beta}(\beta)$ (right) with $e_{max} = 8.342$.

Theorem 4.5 ([7, Theorem 1.6]). *The following statements are equivalent to each other.*

(i) *For any* $U_0 \in (0, \frac{2e_{min}}{b})$, $(\rho, \eta) \in \{(+,-),(-,+)\}$ *there exist* $U \in [-U_0, 0)$, $E \in \mathcal{E}(e_{min}, e_{max})$, $n \in 4\mathbb{N}+2$ $(= \{6, 10, 14, \cdots\})$ *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)

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

Example 4.6 ([7, Figure 2]). In the same exact solution as in Example 3.5 let us take e_{max} to be 6.643, 8.342. In these cases $\frac{e_{min}}{e_{max}} \leq \frac{1}{6.643} < \sqrt{17 - 12\sqrt{2}}$. According to Theorem 4.5, there is a chance that we can find a one-particle Hamiltonian in $\mathcal{E}(e_{min}, e_{max})$ so that the phase boundary has a SPI. By plotting the graphs we can observe that the exact solution with $e_{max} = 6.643, 8.342$ has a rising SPI, a falling SPI respectively. Theorem 4.4 implies that HOPTs must be happening there.

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