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Finite-size Energy of Non-interacting Fermi Gases

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Abstract We study the asymptotics of the difference of the ground-state energies of two non-interacting N-particle Fermi gases in a finite volume of length L in the thermodynamic limit up to order $1/L$. We are particularly interested in subdominant terms proportional to $1/L$, called finite-size energy. In the nineties (Affleck, Nuc. Phys. B **58**, 35–41 1997; Zagoskin and Affleck, J. Phys. A **30**, 5743–5765 1997) claimed that the finite-size energy is related to the decay exponent occurring in Anderson's orthogonality. We prove that the finite-size energy depends on the details of the thermodynamic limit and is therefore non-universal. Typically, it includes an additional linear term in the scattering phase shift.

Keywords Schrödinger operators · Scattering phase shift · Spectral asymptotics

Mathematics Subject Classifications (2010) Primary 81Q10; Secondary 34L25

1 Introduction

Given two non-interacting N-particle Fermi gases, which differ by a local scattering potential, and are confined to the finite interval $(0, L) \subset (0, \infty)$, one can ask for

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two intimately connected asymptotics. The first one is the asymptotics of the scalar product of the two ground states $\langle \Phi_L^N, \Psi_L^N \rangle$, which we call the ground-state overlap in the sequel. The second related question is the asymptotics of the difference of the ground-state energies $E_L'^N - E_L^N$. Both in the thermodynamic limit at some given Fermi energy E, i.e. $N/L \to \rho(E) > 0$. Here, ρ is the integrated density of states of the unperturbed one-particle Schrödinger operator. These asymptotics are related to physical situations where a sudden change by a static scattering potential occurs, e.g. the Fermi edge singularity or the Kondo effect, see [2].

On the one hand, [3] claims in the case of a Dirac-δ perturbation that the ground-state overlap vanishes as

$$\langle \Phi_L^N, \Psi_L^N \rangle \sim L^{-\zeta(E)/2}, \tag{1.1}$$

where

$$\zeta(E) := \frac{1}{\pi^2}\delta^2(\sqrt{E}) \tag{1.2}$$

and δ is equal to the s-wave scattering phase shift. For a proof of this see [10]. It turns out that the decay exponent $\zeta(E)$ is independent of the particular thermodynamic limit chosen, at least in the case of a Dirac-δ perturbation. In more general settings only upper bounds on the ground-state overlap are known, see [7–9, 14, 15]. In the physics literature the behaviour (1.1) is referred to as Anderson's orthogonality catastrophe.

On the other hand, restricting ourselves to systems on the half-axis and the family of thermodynamic limits

$$\frac{N}{L} + \frac{a}{L} = \rho(E), \tag{1.3}$$

where $a \in \mathbb{R}$ is a parameter, the difference of the ground-state energies admits the asymptotics

$$E_L'^N - E_L^N = \int_{-\infty}^{E} \mathrm{d}x\, \xi(x) + \frac{\sqrt{E}\pi}{L} x_{FS}^a(E) + \mathrm{o}\Big(\frac{1}{L}\Big) \tag{1.4}$$

as $N, L \to \infty$ such that (1.3) holds. Here, ξ is the spectral shift function for the pair of the corresponding infinite-volume one-particle Schrödinger operators. In the physics literature the first term is sometimes called the Fumi term and $x_{FS}^a(E)$ the finite-size correction or energy, see [1]. For models on the half line with a local perturbation, the finite-size correction $x_{FS}^a(E)$ appearing in the energy difference is claimed to be closely related to the decay exponent $\zeta(E)$ occurring in Anderson's orthogonality, see [1, 2, 19].

In this note we give a short and elementary proof of the correct asymptotics of the difference of the ground-state energies for systems on the half axis which differ by a short-range scattering potential in the thermodynamic limit, see Theorem 2.2. The proof also applies for a perturbation by a Dirac-δ perturbation. It turns out that the finite-size energy $x_{\mathrm{FS}}^a(E)$ is non-universal and depends on the particular choice of the parameter a in the thermodynamic limit in (1.3). Moreover, there is precisely one choice of the particle number and system size, i.e.

$a = 1/2$ in (1.3), such that the finite-size energy is equal to the Anderson exponent (1.2). This particular choice was also used in a computation of the finite-size energy in [19, App. A]. However, for other choices of the thermodynamic limit an additional linear term in the spectral shift function, or equivalently in the scattering phase shift occurs, see Corollary 2.4 below. In contrast, it is proved in [10] that the decay exponent $\zeta(E)$ in (1.1) is independent of the choice of the constant a in the thermodynamic limit (1.3). Thus, we doubt a fundamental connection between the finite-size energy (1.4) and the decay exponent in Anderson's orthogonality (1.1).

2 Model and Results

We consider a measurable non-negative potential $V \geq 0$ on the half line $(0, \infty)$ satisfying

$$\int_0^\infty dx\, V(x) \left(1 + x^2\right) < \infty. \tag{2.1}$$

Moreover, let $L > 1$ and $-\Delta_L$ be the negative Laplacian on the interval $(0, L)$ with Dirichlet boundary conditions. Then, we define the finite-volume one-particle Schrödinger operators

$$H_L := -\Delta_L \qquad \text{and} \qquad H_L' := -\Delta_L + V. \tag{2.2}$$

Here, V is understood as its canonical restriction to the interval $(0, L)$. These operators are densely defined and self-adjoint operators on the Hilbert space $L^2((0, L))$. Both have compact resolvents and thus admit an ONB of eigenfunctions. We denote the corresponding non-decreasing sequences of eigenvalues, counting multiplicities, by $\lambda_1^L \leqslant \lambda_2^L \leqslant \cdots$ and $\mu_1^L \leqslant \mu_2^L \leqslant \cdots$. Note that $\lambda_n^L = \left(\frac{n\pi}{L}\right)^2$, $n \in \mathbb{N}$, see e.g. [16]. Moreover, we write $H := -\Delta$ and $H' := -\Delta + V$ for the corresponding infinite-volume operators on $L^2((0, \infty))$ with Dirichlet boundary conditions at the origin.

Given $N \in \mathbb{N}$, the induced (non-interacting) finite-volume fermionic N-particle Schrödinger operators $\hat{H}_L$ and $\hat{H}_L'$ act on the totally antisymmetric subspace $\bigwedge_{j=1}^N L^2((0, L))$ of the N-fold tensor product space and are given by

$$\hat{H}_L^{(\prime)} := \sum_{j=1}^N I \otimes \cdots \otimes I \otimes H_L^{(\prime)} \otimes I \otimes \cdots \otimes I, \tag{2.3}$$

where the index j determines the position of $H_L^{(\prime)}$ in the N-fold tensor product of operators. The corresponding ground-state energies are given by the sum of the N smallest eigenvalues

$$E_L^N := \sum_{k=1}^N \lambda_k^L \quad \text{and} \quad E_L'^N := \sum_{j=1}^N \mu_j^L. \tag{2.4}$$

We are interested in the difference of the ground state energies in the thermodynamic limit at a given *Fermi energy* $E > 0$. Thus, given $E > 0$ and the number of particles $N \in \mathbb{N}$, we choose the system length L such that

$$\frac{N}{L} \to \frac{\sqrt{E}}{\pi} =: \rho(E), \tag{2.5}$$

where ρ is the integrated density of states of the infinite-volume operator H.

For $k > 0$ we denote by $\delta(k)$ the scattering phase shift corresponding to the pair of operators H and H' at the energy $k^2 > 0$. Since $V \geq 0$, the phase shift is non-positive, i.e. for $k > 0$

$$\delta(k) \leq 0. \tag{2.6}$$

Then, the scattering matrix for the pair H and H' at the energy E equals $S(E) = \exp\big(2i\delta(\sqrt{E})\big)$. Note that on the half line, the scattering matrix is just a complex number of modulus 1. For a definition of the phase shift see e.g. Appendix A, [17, Chapter. XI.8] or [6].

Remark 2.1. (i) Let ξ be the spectral shift function for the pair of operators H and H'. Then, we have the identity [5]

$$\frac{1}{\pi}\delta(\sqrt{E}) = -\xi(E), \tag{2.7}$$

for every $E > 0$.

(ii) We define for $E > 0$

$$\zeta(E) := \frac{1}{\pi^2}\delta^2(\sqrt{E}). \tag{2.8}$$

This constant equals the decay exponent found in [10] which determines the asymptotics of the exponent in Anderson's orthogonality, i.e. the asymptotics (1.1) of the scalar product of the ground states of the pair of operators $\hat{H}_L$ and $\hat{H}_L^{(\prime)}$ in the thermodynamic limit.

Using the notation of Remark 2.1, our main result is the following:

Theorem 2.2. *For all Fermi energies $E > 0$ the difference of the ground-state energies admits the asymptotics*

$$\begin{aligned} E_L'^N - E_L^N &= -\frac{1}{\pi}\int_0^{\left(\frac{N\pi}{L}\right)^2} \mathrm{d}x\, \delta(\sqrt{x}) + \frac{\sqrt{E}}{L}\Big(-\delta(\sqrt{E}) + \frac{1}{\pi}\delta^2(\sqrt{E})\Big) + \mathrm{o}\Big(\frac{1}{L}\Big) \\ &= \int_0^E \mathrm{d}x\, \xi(x) + \int_E^{\left(\frac{N\pi}{L}\right)^2} \mathrm{d}x\, \xi(x) + \frac{\sqrt{E}\pi}{L}\big(\xi(E) + \zeta(E)\big) + \mathrm{o}\Big(\frac{1}{L}\Big) \end{aligned} \tag{2.9}$$

as $N, L \to \infty$, and $\frac{N}{L} \to \frac{\sqrt{E}}{\pi}$.

Remark 2.3. Since ξ is continuous, see Lemma 3.2 below,

$$\int_E^{\left(\frac{N\pi}{L}\right)^2} \mathrm{d}x\, \xi(x) = \left(\left(\frac{N\pi}{L}\right)^2 - E\right)\xi(E) + \mathrm{o}\left(\left(\frac{N\pi}{L}\right)^2 - E\right) \tag{2.10}$$

as $N, L \to \infty$, and $\frac{N}{L} \to \frac{\sqrt{E}}{\pi} > 0$. This immediately implies that the asymptotics depends on the rate of convergence of the thermodynamic limit and that the finite-size energy defined in (1.4) is non-universal. In general, the first-order correction to the difference of the ground-state energies may even be L dependent.

Remark 2.3 implies for the particular family of thermodynamic limits considered in the introduction:

Corollary 2.4 (Finite-size energy)**.** *For a given Fermi energy $E > 0$, some particle number $N \in \mathbb{N}$ and $a \in \mathbb{R}$ we choose the system length L such that*

$$\frac{N + a}{L} := \frac{\sqrt{E}}{\pi}. \tag{2.11}$$

Then, the $1/L$-correction in (2.9), which is called the finite-size energy introduced in (1.4), is

$$x^a_{FS}(E) = \big(1 - 2a\big)\xi(E) + \zeta(E). \tag{2.12}$$

Thus,

(i) *for the particular choice $a = \frac{1}{2}$ the finite-size energy is*

$$x_{FS}(E) = \zeta(E), \tag{2.13}$$

(ii) *whereas for the choice $a = 0$ the finite-size energy equals*

$$x_{FS}(E) = \xi(E) + \zeta(E). \tag{2.14}$$

Remark 2.5. (i) In our case of $V \geq 0$ the integrals in Theorem 2.2 may start from 0, since $\delta(x) = 0$ for $x \leq 0$.

(ii) The first term in the expansion is not surprising since

$$E'^N_L - E^N_L = \int_{-\infty}^{E} \mathrm{d}x\, \xi_L(x) + \mathrm{o}\,(1)\,, \tag{2.15}$$

where ξ_L is the finite-dimensional spectral shift function and

$$\int_{-\infty}^{E} \mathrm{d}x\, \xi_L(x) \to \int_{-\infty}^{E} \mathrm{d}x\, \xi(x) \tag{2.16}$$

as $L \to \infty$, see [11] or [4] for definitions and details.

(iii) The same result with the completely analogous proof holds also for a Dirac-δ perturbation or s-wave scattering in three dimensions which is considered in [10]. In the special case of the Neumann and Dirichlet Laplacian $H := -\Delta^N$

and $H' := -\Delta^D$ on $L^2((0,\infty))$ the proof is even simpler since the phase shift is energy independent

$$\delta(\sqrt{E}) = \frac{\pi}{2} \tag{2.17}$$

and one easily obtains the a-dependence in Corollary 2.4.

(iv) We choose $V \geq 0$ since we want to avoid bound states or zero-energy resonances. Moreover, the integrability assumption (2.1) on V ensures sufficient regularity of the phase shift δ.

(v) Our result allows also a conclusion for the same problem on $\mathbb{R}$ with a symmetric perturbation V because in this case the problem is reduced to two problems on the half axis with either Neumann or Dirichlet boundary condition at the origin.

3 Proof of Theorem 2.2

We start with a lemma relating the eigenvalues of the pair of finite-volume operators.

Lemma 3.1. *Let δ be the phase shift for the pair of operators H and H' then the nth eigenvalues of H_L and H'_L satisfy*

$$\sqrt{\mu_n} = \sqrt{\lambda_n} - \frac{\delta(\sqrt{\mu_n})}{L} + \mathrm{o}\Big(\frac{1}{L^2}\Big), \tag{3.1}$$

where the error depends only on the potential V.

This follows directly from introducing Prüfer variables in the theory of Sturm-Liouville operators.

We have to investigate the behaviour of δ at $k = 0$ to obtain suitable error estimates.

Lemma 3.2. *Let δ be the phase shift corresponding to the operators H and H'. Then, $\delta \in C^2((0,\infty))$ and there exists a constant c, depending on the potential V, such that for all $k > 0$*

(i) $|\delta(k)| \leq c \min\{k, \frac{1}{k}\}$*, in particular* $\delta \in L^\infty((0,\infty))$.

(ii) $\delta' \in L^\infty((0,\infty))$,

(iii) $|\delta''(k)| \leq \frac{c}{k}$.

Moreover,

(iv) *we have the following expansion of the phase shift*

$$\delta(\sqrt{\mu_n}) = \delta(\sqrt{\lambda_n}) - \frac{\delta'(\sqrt{\lambda_n})\delta(\sqrt{\lambda_n})}{L} + \frac{F(\sqrt{\lambda_n})}{L^2}, \tag{3.2}$$

where the remainder term obeys for $x > 0$

$$\big|F(x)\big| \le c\Big(\frac{1}{x} + 1\Big) \tag{3.3}$$

for some constant c depending on the potential V.

Lemma 3.1 and 3.2 are well known to experts in the theory of Sturm-Liouville operators. Unfortunately, we did not find a precise reference. For convenience, we prove both results in Appendix A. The third ingredient to the proof of Theorem 2.2 is the following:

Lemma 3.3. *(Euler-MacLaurin)*

(i) *Let $f \in C^1((0,\infty))$ then*

$$\frac{1}{L}\sum_{n=1}^{N} f\left(\frac{n}{L}\right) = \int_0^{\frac{N}{L}} \mathrm{d}x\ f(x) + \mathrm{O}\Big(\frac{N}{L^2}\Big)\|f'\|_{L^\infty\left((0,\frac{N}{L})\right)}. \tag{3.4}$$

(ii) *Let $f \in C^2((0,\infty))$ with $f'' \in L^\infty((0,\infty))$ then*

$$\frac{1}{L}\sum_{n=1}^{N} f\left(\frac{n}{L}\right) = \int_0^{\frac{N}{L}} \mathrm{d}x\ f(x) + \frac{1}{2L}\int_0^{\frac{N}{L}} \mathrm{d}x\ f'(x) + \mathrm{O}\Big(\frac{N}{L^3}\Big). \tag{3.5}$$

The proof of this lemma is elementary, see also [13, Chapter XIV].

Proof of Theorem 2.2 Using Lemma 3.1, we obtain

$$\sum_{n=1}^{N}\big(\mu_n - \lambda_n\big) = \sum_{n=1}^{N}\Big(-\frac{2\sqrt{\lambda_n}\delta(\sqrt{\mu_n})}{L} + \frac{\delta^2(\sqrt{\mu_n})}{L^2}\Big) + \mathrm{o}\Big(\frac{N}{L^2}\Big) \tag{3.6}$$

On the other hand Lemma 3.2 (iv) provides

$$\begin{aligned}(3.6) = &\sum_{n=1}^{N}\Big(-\frac{2\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L} + \frac{2\delta'(\sqrt{\lambda_n})\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L^2} + \frac{\delta^2(\sqrt{\lambda_n})}{L^2}\Big)\\ &+\frac{1}{L^3}\sum_{n=1}^{N} G\big(\sqrt{\lambda_n}\big) + \mathrm{o}\big(\frac{N}{L^2}\big),\end{aligned} \tag{3.7}$$

where

$$\begin{aligned}G(x) = \Big(&-2\delta'(x)\delta^2(x) - 2xF(x) + \frac{1}{L}\big((\delta'(x)\delta(x))^2 + 2\delta(x)F(x)\big)\\ &-\frac{2}{L^2}F(x)\delta'(x)\delta(x) + \frac{1}{L^3}F^2(x)\Big).\end{aligned} \tag{3.8}$$

Since $\lambda_n = \left(\frac{n\pi}{L}\right)^2$, $\frac{N}{L} \to \frac{\sqrt{E}}{\pi}$, using Lemma 3.2 (i)-(iii) and (3.3), we obtain for the error

$$\frac{1}{L^3}\sum_{n=1}^{N} G\big(\sqrt{\lambda_n}\big) = \mathrm{O}\Big(\frac{1}{L^2}\Big). \tag{3.9}$$

Note that by Lemma 3.2 the function $f : x \mapsto x\delta(x)$ fulfills the assumptions of Lemma 3.3 (ii). Thus, we compute

$$\begin{aligned}\sum_{n=1}^{N} -\frac{2\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L} &= -\frac{1}{L}\sum_{n=1}^{N} 2\delta\left(\frac{n\pi}{L}\right)\frac{n\pi}{L}\\ &= -\int_0^{\frac{N}{L}} \mathrm{d}x\, 2\delta(x\pi)(x\pi) - \frac{1}{L}\int_0^{\frac{N}{L}} \mathrm{d}x\ (\delta(x\pi)(x\pi))' + \mathrm{O}\Big(\frac{N}{L^3}\Big)\\ &= -\frac{1}{\pi}\int_0^{(\frac{N\pi}{L})^2} \mathrm{d}x\, \delta(\sqrt{x}) - \frac{1}{L}\delta(\sqrt{E})\sqrt{E} + \mathrm{o}\Big(\frac{1}{L}\Big),\end{aligned} \tag{3.10}$$

where we used in the last equality the convergence $\frac{N}{L} \to \frac{\sqrt{E}}{\pi}$ and the continuity of δ. Using Lemma 3.2 we see that $g : x \mapsto x\delta(x)\delta'(x)$ satisfies the assumptions of Lemma 3.3 (i) with $\|g'\|_{L^\infty\left((0,\frac{N}{L})\right)} \le c(1+\frac{N}{L})$. Therefore,

$$\begin{aligned}\sum_{n=1}^{N} \frac{2\delta'(\sqrt{\lambda_n})\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L^2} &= \frac{1}{L}\left(\frac{1}{L}\sum_{n=1}^{N} 2\delta'\left(\frac{n\pi}{L}\right)\delta\left(\frac{n\pi}{L}\right)\frac{n\pi}{L}\right)\\ &= \frac{1}{L}\int_0^{\frac{N}{L}} \mathrm{d}x\, 2\delta'(x\pi)\delta(x\pi)(x\pi) + \mathrm{O}\Big(\frac{N}{L^3}\Big)\Big(1+\frac{N}{L}\Big)\\ &= \frac{1}{L\pi}\Big(\delta^2(\sqrt{E})\sqrt{E} - \int_0^{\frac{N}{L}} \mathrm{d}x\, \delta^2(x\pi)\pi\Big) + \mathrm{o}\Big(\frac{1}{L}\Big),\end{aligned} \tag{3.11}$$

where we used integration by parts, the convergence $\frac{N}{L} \to \frac{\sqrt{E}}{\pi}$ and the continuity of δ in the last line. Lemma 3.2 yields the assumptions of Lemma 3.3 (i) for $h : x \mapsto \delta^2(x)$ with $h' \in L^\infty((0,\infty))$. Thus,

$$\begin{aligned}\sum_{n=1}^{N} \frac{\delta^2(\sqrt{\lambda_n})}{L^2} &= \frac{1}{L}\left(\frac{1}{L}\sum_{n=1}^{N} \delta^2\left(\frac{n\pi}{L}\right)\right)\\ &= \frac{1}{L}\int_0^{\frac{N}{L}} \mathrm{d}x\, \delta^2(x\pi) + \mathrm{O}\Big(\frac{1}{L^2}\Big).\end{aligned} \tag{3.12}$$

Summing up (3.10), (3.11), (3.12) and (3.6), (3.9) give the claim. □

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Appendix A: Prüfer Variables and the Phase Shift

Let $k > 0$. We consider the eigenvalue problem on $(0, \infty)$

$$-u'' + Vu = k^2 u, \qquad u(0) = 0. \tag{A.1}$$

Introducing Prüfer variables

$$u(x) = \rho_u(x)\sin(\theta_k(x)) \qquad u'(x) = k\rho_u(x)\cos(\theta_k(x)), \tag{A.2}$$

(A.1) is equivalent to the system

$$\theta_k' = k - \frac{1}{k} V \sin^2(\theta_k), \qquad \theta_k(0) = 0, \tag{A.3}$$

$$\rho_u' = \frac{V\sin(2\theta_k)}{2k}\rho_u, \tag{A.4}$$

see e.g. [18, Sec. 14.4]. We call θ_k the Prüfer angle. Using the Banach fixed-point theorem, there exist absolutely continuous solutions θ_k and $\rho_u > 0$ of (A.3) and (A.4). Moreover, the solution θ_k is unique. We denote by

$$\delta_k(x) := \theta_k(x) - kx, \quad \text{where } k, x > 0 \tag{A.5}$$

the phase shift function, Then, for $k > 0$ the scattering phase shift δ is defined by

$$\lim_{x\to\infty} \delta_k(x) := \delta(k). \tag{A.6}$$

Therefore, integrating (A.3) implies

$$\delta(k) = -\frac{1}{k}\int_0^\infty \mathrm{d}t\, V(t)\sin^2(\theta_k(t)). \tag{A.7}$$

The non-linear ODE (A.3) is sometimes called the variable-phase equation, see e.g. [6] or [17, Thm. XI.54]. We did not choose the standard Prüfer variables. But with the choice (A.2) it is particularly easy to compare the Prüfer angle with the phase-shift function and in turn with the phase shift. This was also used in [12]. We continue with some elementary properties of the Prüfer angle, respectively of the phase-shift function for perturbations $V \geqslant 0$.

Proposition A.1. *Let $V \geqslant 0$, $k > 0$ and fix $x > 0$. Then,*

(i) *$\theta_k(x)$ is non-negative, moreover,*

$$0 \le \theta_k(x) \le kx, \tag{A.8}$$

(ii) *we have*

$$\lim_{k\to 0} \theta_k(x) = 0, \qquad \lim_{k\to\infty} \theta_k(x) = \infty, \tag{A.9}$$

(iii) *the functions* $k \mapsto \theta_k(x)$ *and* $k \mapsto \delta_k(x)$ *are twice differentiable, i.e.*

$$\theta_{(\cdot)}(x),\ \delta_{(\cdot)}(x) \in C^2((0,\infty)), \tag{A.10}$$

where $\frac{\partial}{\partial k}\theta_k$ *satisfies*

$$\frac{\partial}{\partial k}\theta_k(x) = \int_0^x \mathrm{d}t\, \frac{\rho^2(t)}{\rho^2(x)}\Big(1 + \frac{V(t)\sin^2(\theta_k(t))}{k^2}\Big) \geq 0. \tag{A.11}$$

Proof of Proposition A.1 The first inequality in (i) follows from integrating (A.11) with the initial condition $\theta_k(0) = 0$ for all $k > 0$. The second inequality follows from $V \geqslant 0$ and the ODE (A.3).

The first equality in (ii) is a consequence of (i). The second equality follows directly from the ODE.

Let $u(x,k)$ be a non-trivial solution of (A.1). Standard results provide that u and u' are analytic functions in the parameter k [18, Kor. 13.3]. Note that u and u' do not have the same zeros. Since $\tan\big(\theta_k(x) = ku(x,k)/u'(x,k)\big)$ for $u'(x,k) \neq 0$ and $\operatorname{cotan}\big(\theta_k(x)\big) = u'(x,k)/(ku(x,k))$ for $u(x,k) \neq 0$, the properties (A.10) follow from the analyticity of u. We compute

$$\begin{aligned}\Big(\rho^2\frac{\partial}{\partial k}\theta\Big)_x &= 2\rho\rho_x\frac{\partial}{\partial k}\theta + \rho^2\frac{\partial}{\partial k}\theta_x\\ &= 2\rho\rho_x\frac{\partial}{\partial k}\theta + \rho^2\frac{\partial}{\partial k}\Big(k - \frac{V\sin^2(\theta)}{k}\Big)\\ &= 2\rho\rho_x\frac{\partial}{\partial k}\theta + \rho^2\Big(1 + \frac{V\sin^2(\theta)}{k^2} - \frac{V\sin(2\theta)}{k}\frac{\partial}{\partial k}\theta\Big)\\ &= \rho^2\Big(1 + \frac{V\sin^2(\theta)}{k^2}\Big).\end{aligned} \tag{A.12}$$

Integrating the latter yields (A.11). This computation is adopted from [18, Lem. 14.16]. □

Proof of Lemma 3.1 Let $\mu > 0$. Consider the eigenvalue equation on $[0, L]$

$$-u'' + Vu = \mu u, \qquad u(0) = 0. \tag{A.13}$$

We introduce Prüfer variables according to (A.2). Note that any eigenfunction u of $h_L'^D$ corresponding to an eigenvalue μ has to fulfill $u(L) = 0$ due to the Dirichlet boundary condition at L. Thus, using $\rho_u(x) \neq 0$ for all $x \geq 0$, we obtain $\sin\big(\theta_{\sqrt{\mu}}(L)\big) = 0$. With (A.9) and (A.11) this implies for the nth eigenvalue μ_n of $h_L'^D$

$$\theta_{\sqrt{\mu_n}}(L) = n\pi. \tag{A.14}$$

Therefore, integrating (A.3) yields

$$\sqrt{\mu}_n = \frac{n\pi}{L} + \frac{1}{L\sqrt{\mu}_n}\int_0^L \mathrm{d}t\ V(t)\sin^2\left(\theta_{\sqrt{\mu_n}}(t)\right). \tag{A.15}$$

Now, using $|\sin(x)| \leq |x|$, (A.8), $|\sin(x)| \leq 1$ and (2.1) we obtain

$$\begin{aligned}\frac{1}{\sqrt{\mu_n}}\int_L^\infty \mathrm{d}t\ V(t)\sin^2(\theta_{\sqrt{\mu_n}}(t)) &\leq \int_L^\infty \mathrm{d}t\ V(t)t \\ &\leq \frac{1}{L}\int_L^\infty \mathrm{d}t\ t^2V(t) = \mathrm{o}\Big(\frac{1}{L}\Big).\end{aligned} \tag{A.16}$$

Then, (A.7) and $\sqrt{\lambda_n} = \frac{n\pi}{L}$ give the claim. □

Proof of Lemma 3.2 Part (i) follows from (A.7), (A.8) and (2.1).

Equation (A.10) implies

$$\frac{\partial}{\partial k}\theta_k(x) = \int_0^x \mathrm{d}t\ \frac{\rho^2(t)}{\rho^2(x)}\Big(1 + \frac{V(t)\sin^2(\theta_k(t))}{k^2}\Big). \tag{A.17}$$

The ODE (A.4), (A.8), the elementary inequality $|\sin x| \leq |x|$ and (2.1) imply

$$\Big|\frac{\rho(t)}{\rho(x)}\Big| \leq exp\Big(\int_t^x \mathrm{d}s\ sV(s)\Big) \leq exp\big(\|(\cdot)V\|_1\big) < \infty. \tag{A.18}$$

From this, (A.8) and $|\sin x| \leq |x|$ we infer the existence of a constant c depending on the potential V such that

$$\Big|\frac{\partial}{\partial k}\theta_k(x)\Big| \leq c\,(1+x)\,. \tag{A.19}$$

Then, the above, (A.8) and dominated convergence provide $\delta \in C^1((0,\infty))$ with

$$\big|\delta'(k)\big| \leq c\int_0^\infty \mathrm{d}t\ V(t)\big(1+t+t^2\big). \tag{A.20}$$

The assumptions on the potential give the claim.

Using (A.10), we compute as in the proof of (A.11)

$$\Big(\rho^2\frac{\partial^2}{\partial k^2}\theta\Big)_x = 2\rho^2V\Big(-\frac{\sin^2(\theta)}{k^3} + \frac{\sin(2\theta)\frac{\partial}{\partial k}\theta}{k^2} - \frac{\cos(2\theta)(\frac{\partial}{\partial k}\theta)^2}{k}\Big). \tag{A.21}$$

Using (A.8), $|\sin x| \leq |x|$, (A.18) and (A.19), we see

$$\Big|\frac{\partial^2}{\partial k^2}\theta_k(x)\Big| \leq \frac{\tilde{c}}{k}, \tag{A.22}$$

where $\tilde{c}$ depends on V. Then dominated convergence yields $\delta \in C^2((0,\infty))$ and (A.8) and (A.22) provide

$$\big|\delta''(k)\big| \leq \frac{C}{k}\int_0^\infty \mathrm{d}t\ V(t)\big(1+t+t^2\big) \tag{A.23}$$

for some C depending on the potential V.

To prove (iv) we use Lemma 3.1. Thus,

$$\sqrt{\mu_n} = \sqrt{\lambda_n} + \frac{\delta(\sqrt{\mu_n})}{L} + \mathrm{o}\Big(\frac{1}{L}\Big), \tag{A.24}$$

Since $\delta \in C^2((0,\infty))$ we compute for $x, y \in (0,\infty)$ with $y > x$ and $y = x + \frac{\delta(y)}{L} + \mathrm{o}\big(\frac{1}{L}\big)$

$$\begin{aligned}\Big|\delta(y) - \delta(x) + \frac{\delta'(x)\delta(x)}{L}\Big| &\le \Big|\int_x^y \mathrm{d}t \int_x^t \mathrm{d}s\,\delta''(s)\Big| + |\delta'(x)|\Big|y - x + \frac{\delta(x)}{L}\Big| \\ &\le \frac{1}{x}|y-x|^2 + \frac{\|\delta\|_\infty}{L}\Big|\int_x^y \mathrm{d}t\,\delta'(t) + \mathrm{o}\Big(\frac{1}{L}\Big)\Big|. \end{aligned} \tag{A.25}$$

Using Lemma 3.2 (ii) and once again the recursion relation we obtain

$$\Big|\delta(y) - \delta(x) + \frac{\delta'(x)\delta(x)}{L}\Big| \le \Big(\frac{1}{x} + 1\Big)\mathrm{O}\Big(\frac{1}{L^2}\Big). \tag{A.26}$$

The claim follows from setting $x := \lambda_n$ and $y := \mu_n$. □

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