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Asymptotics of the Interband Light Absorption Coefficient near the Band Edge for an Alloy-Type Model

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We find the asymptotics of the interband light absorption coefficient of an alloy-type model in the case when the ground-state energies of the electron and the hole Hamiltonians are finite.

KEY WORDS: Light absorption; Lifshitz tails; random Schrödinger operators; doped semiconductors; density of states.

1. INTRODUCTION

In this paper we continue to study the interband light absorption coefficient (ILAC) (see papers Kirsch and Pastur,[5] and Khoruzhenko, Kirsch, and Pastur[2] for previous results). The ILAC is an important characteristics of semiconductors, which in a certain approximation can be defined as follows.

Let $V_\omega(x)$ be an ergodic field in $\mathbb{R}^\nu$ and $H_\omega^\pm = -\frac{1}{2}\Delta \pm V_\omega$ are the Schrödinger operators acting in $L^2(\mathbb{R}^\nu)$. Denote

$$\hat{A}_\Lambda(\lambda) = \frac{1}{|\Lambda|} \sum_{\substack{\lambda_n^+ \in \sigma(H_\omega^+) \\ \lambda_m^- \in \sigma(H_\omega^-) \\ \lambda_n^+ + \lambda_m^- + E_g \leqslant \lambda}} |(\varphi_{\lambda_n^+}, \varphi_{\lambda_m^-})|^2 \tag{1}$$

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where $(\cdot, \cdot)$ is the inner product in $L^2(\mathbb{R}^\nu)$. E_g is the distance gap between the valence and the conduction band. $\lambda_n^\pm$ and $\varphi_{\lambda_n^\pm}$ are the eigenvalues and orthonormalized eigenfunctions respectively of the operators $H_\Lambda^\pm$, which denote $H_\omega^\pm$ restricted to the cube Λ with appropriate (e.g., Dirichlet) boundary conditions. These Hamiltonians describe the motions of electrons and holes in the conduction and valence bands under the influence of the random (impurity) potential V_ω. The energy levels $\lambda_n^\pm$ are counted from the bottom of the respective band. For simplicity we consider only the case of equal effective masses of electrons and holes. The absorption of light of frequency f, i.e., of photons of energy $E = hf$, by the semiconductor is possible only if

$$hf = \lambda_n^+ + \lambda_m^- + E_g$$

Now we define the ILAC by

$$A(\lambda) := \lim_{\Lambda \uparrow \mathbb{R}^\nu} \hat{A}_\Lambda(\lambda) \tag{2}$$

For its Laplace transform we get (Kirsch[3], Chapter 10)

$$\tilde{A}(t) = \int_{\mathbb{R}^\nu} p(t, x)^2 \, \mathbb{E}_{0,0}^{t,x} \otimes \mathbb{E}_{0,x}^{t,0} \otimes E\left(\exp\left(-\int_0^t (V_\omega(\beta(s)) - V_\omega(\beta'(s)))\, ds\right)\right) \tag{3}$$

Here $p(t, x)$ denotes $(2\pi t)^{-\nu/2} \exp(-|x|^2/(2t))$. $\mathbb{E}_{0,0}^{t,x}$ is the expectation for the Brownian bridge $\beta(s)$ with starting time 0, end-time t, starting point 0 and end-point x. $\mathbb{E}_{0,x}^{t,0}$ denotes the corresponding expectation for $\beta'(s)$, E means the expectation for V_ω^+, V_ω^-.

In this article the asymptotics of the ILAC are estimated for the following alloy type potential:

Definition 1. Let

$$V_\omega := \sum_{i \in \mathbb{Z}^\nu} \xi_i f(x - i) \tag{4}$$

Where ν denotes the dimension of space, ξ_i are integrable i.i.d. random variables with

$$-\infty < \xi_{\min} < \xi_{\max} < \infty$$

and there are constants C, $N > 0$, $\varepsilon_{\min}$, $\varepsilon_{\max}$ such that[4]

$$P([\xi_{\min}, \varepsilon)) \geqslant c(\varepsilon - \xi_{\min})^N \qquad \text{for all} \quad \xi_{\min} \leqslant \varepsilon < \varepsilon_{\min} \tag{5}$$

$$P((\varepsilon, \xi_{\max}]) \geqslant c(\xi_{\min} - \varepsilon)^N \qquad \text{for all} \quad \xi_{\max} \geqslant \varepsilon > \varepsilon_{\max} \tag{6}$$

For simplicity let f bounded.
Then we call V_ω an alloy type potential.

We have to differ two types of alloy type potentials.

Definition 2. We say that an alloy type potential $V_\omega := \sum_{i \in \mathbb{Z}^\nu} \xi_i f(x-i)$ has

1. slow decay, if

$$\infty > M \geqslant f \geqslant 0, \qquad \lim_{|x| \to \infty} \frac{f(x)}{|x|^{-\alpha}} = \gamma > 0 \qquad \text{for} \quad \nu < \alpha \leqslant \nu + 2 \tag{7}$$

2. fast decay, if

$$\infty > M \geqslant f \geqslant 0, \qquad \lim_{|x| \to \infty} \frac{f(x)}{|x|^{-(\nu+2)}} = 0 \tag{8}$$

For these alloy type potentials V_ω, the groundstates $E_0^\pm$ of

$$H_\omega^\pm = -\tfrac{1}{2}\Delta \pm V_\omega$$

are both bigger than $-\infty$. This is in contrast to the models considered in ref. 5.

[4] $\xi_{\min} := \inf\{r \mid P((-\infty, r] > 0)\}$, $\xi_{\max} = \sup\{r \mid P([r, \infty) > 0)\}$, where P denotes the probability distribution of the ξ_i.

We state

Theorem 3. Let $A(\lambda)$ the ILAC of an alloy type potential. Then

1.

$$\lim_{\lambda \downarrow (E_0^+ + E_0^-)} \frac{\ln(-\ln A(\lambda))}{\ln(\lambda - (E_0^+ + E_0^-))} = -\frac{\nu}{\alpha - \nu} \tag{9}$$

in the case of slow decay.

2.

$$\lim_{\lambda \downarrow (E_0^+ + E_0^-)} \frac{\ln(-\ln A(\lambda))}{\ln(\lambda - (E_0^+ + E_0^-))} = -\frac{\nu}{2} \tag{10}$$

in the case of fast decay.

The result is in accordance with the conjecture (Kirsch[3], Section 10.4)

$$\ln \tilde{A}(t) \sim \ln(\tilde{N}^+(t) \cdot \tilde{N}(t)) \qquad \text{for} \quad t \to \infty$$

where $\tilde{A}(t)$ denotes the Laplace transform of the ILAC and $\tilde{N}^{\pm}(t)$ the Laplace transforms of the integrated density of states IDS of $H_\omega^{\pm}$. The asymptotics of the IDS $N^{\pm}(\lambda)$ of $H_\omega^{\pm}$ is determined directly in the article by Kirsch and Simon[7] (observe the following section).

The connection between the ILAC $A(\lambda)$ or rather the IDS $N(\lambda)$ and their Laplace transforms is given by the tauberian theorems in Fukushima.[1]

2. PREPARATION AND SOME NOTATION

First split the potential

$$V_\omega(x) = \underbrace{\sum_{i \in \mathbb{Z}^\nu} \xi_{\min} f(x-i)}_{=:\, V_{\min}(x)} + \underbrace{\sum_{i \in \mathbb{Z}^\nu} \underbrace{(\xi_i - \xi_{\min})}_{=:\, \xi_i^+} f(x-i)}_{=:\, V_\omega^+(x)}$$

$$-V_\omega(x) = \underbrace{-\sum_{i\in\mathbb{Z}^\nu} \xi_{\max} f(x-i)}_{=:\,V_{\max}(x)} + \underbrace{\sum_{i\in\mathbb{Z}^\nu} \underbrace{(\xi_{\max}-\xi_i)}_{=:\,\xi_i^-} f(x-i)}_{=:\,V_\omega^-(x)}$$

So $V_\omega^\pm$ are non negative and bounded. Now define for V_b^a with

$$H_b^a := -\tfrac{1}{2}\Delta + V_b^a$$

$$a \in \{+;-\}, \qquad b=\omega \text{ or min etc.}$$

and observe (Kirsch[3], Chapter 6)

$$\inf\sigma(H_\omega^+) = \inf\sigma(H_{\min}) = E_0^+ > -\infty$$

$$\inf\sigma(H_\omega^-) = \inf\sigma(H_{\max}) = E_0^- > -\infty$$

We set for abbreviation

$$V_{\omega,u} := V_\omega(\cdot+u), \quad V_0^+ := V_{\min} - E_0^+, \qquad V_0^- := -V_{\max} - E_0^-$$

Then

$$\tilde{A}^*(t) = \int_{\mathbb{R}^\nu} dx\, p(t,x)^2\, \mathbb{E}_{0,0}^{t,x} \otimes \mathbb{E}_{0,x}^{t,0} \otimes E \otimes \int_{C_0} du$$
$$\times\left[\exp\left(-\int_0^t V_{0,u}^+(\beta(s))\,ds\right)\exp\left(-\int_0^t V_{0,u}^-(\beta'(s))\,ds\right)\right.$$
$$\left.\times\exp\left(-\int_0^t (V_{\omega,u}^+(\beta(s)) + V_{\omega,u}^-(\beta'(s)))\,ds\right)\right] \tag{11}$$

must be estimated (Kirsch,[3] Chapter 10). In (11) C_0 is the unit cube $\{x\in\mathbb{R}\nu \mid 0\leqslant x_i<1,\, i=1,\dots,\nu\}$. We need the integral over C_0 here because V_ω is only $\mathbb{Z}^\nu$-ergodic (Kirsch[4]).

The reason why in the above formula $V_{0,u}^+$ and $V_{0,u}^-$ are written instead of $V_{\min,u}$ and $V_{\max,u}$ is that the Tauberian theorem only gives a correspondence between the asymptotics with $t\to\infty$ for the Laplace transform and with $\lambda\downarrow 0$ for the respective right continuous function while we are interested in the asymptotics of $A(\lambda)$ with $\lambda \downarrow (E_0^+ + E_0^-)$. $(E_0^+ + E_0^-)$ is not necessarily equal to zero. Therefore we wrote $\tilde{A}^{\#}$ instead of $\tilde{A}$.

3. THE UPPER BOUND

Theorem 4. There exists

case of slow decay a constant $c_1(\alpha) > 0$, such that

$$\limsup_{t \to \infty} t^{-\nu/\alpha} \ln \tilde{A}^{\#}(t) \leqslant -c_1(\alpha) \tag{12}$$

case of fast decay a constant $c_1 > 0$, such that

$$\limsup_{t \to \infty} t^{-\nu/(\nu+2)} \ln \tilde{A}^{\#}(t) \leqslant -c_1 \tag{13}$$

Proof. We start with

$$\tilde{A}_\Lambda(t) := \operatorname{tr}(e^{-tH_\Lambda^+} e^{-tH_\Lambda^-})$$

where $H_\Lambda^\pm$ denote the Operators $H_\omega^\pm$ restricted to the cube Λ with Dirichlet boundary conditions. By the Hölder inequality for traces (Simon,[11] Theorem 2.8) we get because of the semigroup property of $e^{-tH_\Lambda^\pm}$

$$\tilde{A}_\Lambda(t) \leqslant \sqrt{\operatorname{tr} e^{-2tH_\Lambda^+} \operatorname{tr} e^{-2TH_\Lambda^-}} =: \sqrt{\tilde{N}_\Lambda^+(2t)\, \tilde{N}_\Lambda^-(2t)}$$

By taking expectations and using the Hölder inequality we get

$$E(\tilde{A}_\Lambda(t)) \leqslant \sqrt{E(\tilde{N}_\Lambda^+(2t))\, E(\tilde{N}_\Lambda^-(2t))}$$

Now dividing by $|\Lambda|$ and putting $\limsup_{\Lambda \uparrow \mathbb{R}^\nu}$ on both sides we arrive at (Kirsch,[3] Chapters 9 and 10)

$$\tilde{A}(t) \leqslant \sqrt{\tilde{N} + (2t)\, \tilde{N}^-(2t)}$$

Multiplication with $e^{t(E_0^+ + E_0^-)}$ leads to

$$\tilde{A}^{\#}(t) \leqslant \sqrt{\tilde{N}_{\#}^+(2t)\, \tilde{N}_{\#}^-(2t)} \tag{14}$$

where $\tilde{N}^{\pm}_{\#}(t)$ denote the Laplace transforms of $N^{\pm}(\lambda - E_0^{\pm})$. By Kirsch/Simon[7] we know

$$N^{\pm}(\lambda - E_0^{\pm}) \leqslant e^{-k_1^{\pm}(\alpha)(\lambda - E_0^{\pm})^{-\nu/(\alpha-\nu)}}$$

in the slow decaying case and

$$N^{\pm}(\lambda - E_0^{\pm}) \leqslant e^{-k_1^{\pm}(\lambda - E_0^{\pm})^{-\nu/2}}$$

for an alloy type potential with fast decay. An application of a Tauberian theorem leads to

$$\limsup_{t \to \infty} t^{-\nu/\alpha} \ln \tilde{N}^{\pm}_{\#}(t) \leqslant k_2^{\pm}(\alpha) \tag{15}$$

respectively

$$\limsup_{t \to \infty} t^{-\nu/(\nu+2)} \ln \tilde{N}^{\pm}_{\#}(t) \leqslant k_2^{\pm} \tag{16}$$

With (14) we reach at the desired result. ∎

4. THE LOWER BOUND

Theorem 5. In the case of slow decay

$$\liminf_{t \to \infty} t^{-(\nu/\alpha)-\delta} \ln \tilde{A}^{\#}(t) \geqslant 0 \qquad \text{for all} \quad \delta > 0 \tag{17}$$

holds. If in addition

$$P(\xi_0 = \xi_{\min}), \qquad P(\xi_0 = \xi_{\max}) > 0 \tag{18}$$

is fulfilled, there is a constant $c_2(\alpha) > 0$ with

$$\liminf_{t \to \infty} t^{-\nu/\alpha} \ln \tilde{A}^{\#}(t) \geqslant -c_2(\alpha) \tag{19}$$

In the case of fast decay we get

$$\liminf_{t \to \infty} t^{-\nu/(\nu+2)-\delta} \ln \tilde{A}^{\#}(t) \geqslant 0 \qquad \text{for all} \quad \delta > 0 \tag{20}$$

respectively

$$\liminf_{t \to \infty} t^{-\nu/(\nu+2)} \ln \tilde{A}^{\#}(t) \geqslant -c_2 \tag{21}$$

with some positive constant c_2 if (18) is fulfilled.

It suffices to prove the theorem in the case of slow decay. For the proof in the case of fast decay we first estimate $\tilde{A}^{\#}(t)$ from below by replacing in $V_{\omega}^{\pm} f$ by $f+g$, where g is a bounded, not negative C^{∞}-function with

$$\lim_{|x| \to \infty} \frac{g(x)}{|x|^{-(\nu+2)}} = \gamma > 0$$

for some γ. The proof for the deterministic part does not depend on the behaviour of decay. The reason why we cannot improve the lower bound in the case of fast decay is Lemma 12 or rather Proposition 11 in the proof for the deterministic part. This means that in the case of fast decay we have a combination of the contributions of potential (random) and kinetic (deterministic) energy.

Before we prove Theorem 5 we give a short description of the idea for the solution in the next subsection.

4.1. Motivation of the Solution

The first goal for the decisive random part of the expression (11) is to make the potentials in the integral

$$\int_0^t (V_{\omega,u}^{+}(\beta(s)) + V_{\omega,u}^{-}(\beta'(s)))\, ds$$

independent of s small, in order to replace the integral $\int_0^t \cdots ds$ by the factor t.

For this we restrict the domain of integration of the integrals

$$= \int_{\mathbb{R}^\nu} dx\, p(t,x)^2\, \mathbb{E}_{0,0}^{t,x} \otimes \mathbb{E}_{0,x}^{t,0}$$

How far we may do this shows

Proposition 6. Let $B(s)$ be a Brownian motion started in zero and $\mathbb{P}$ its probability distribution. If $a(t) > 0$ is a monotonically increasing function, there are two constants $c_3, c_4 > 0$ depending only on the dimension such that for all $t > 0$

$$\mathbb{P}(|B(s)| \leqslant a(t) \mid 0 \leqslant s \leqslant t) \geqslant c_3 \exp\left(-c_4 \frac{t}{a^2(t)}\right) \tag{22}$$

By construction

$$\mathbb{P}(|B(s)| \leqslant a(t) \mid 0 \leqslant s \leqslant t)$$
$$= \int_{|y| \leqslant a(t)} p(t, y)\, \mathbb{P}^{t, y}_{0, 0}(|\beta(s)| \leqslant a(t) \mid 0 \leqslant s \leqslant t)\, dy$$

holds, where $\mathbb{P}^{t, y}_{0, 0}$ denotes the probability distribution governing the Brownian bridge $\beta(s)$ with starting time 0, end-time t, starting point 0 and end-point y.

For a proof see, e.g., Kirsch,(3) Section 9.5, Lemma 3.

Proposition 6 allows to restrict the domain of integration for the two Brownian bridges such that they do not leave for nearly the whole time t the balls with radius $t^{1/\alpha}$ centered by their starting point 0 respectively x, to make sure that the remaining part of the probability has still the desired asymptotic.

By a suitable restriction of the domain of integration over dx we may suppose that the two balls even with doubled radius do not overlap. This is necessary as the random variables ξ_i^+ and ξ_i^- belonging to the potentials $V^+_{\omega, u}$ respectively $V^-_{\omega, u}$ are coupled. If ξ_i^+ is very small in the interval $[\xi_{\min}, \xi_{\max}]$, then ξ_i^- is very big there and vice versa.

Both potentials $V^+_{\omega, u}$ and $V^-_{\omega, u}$ are defined in a way, that one has at each point i of the lattice $\mathbb{Z}^\nu$ a random charge represented by the random variable ξ_i^+ respectively ξ_i^-, whose potential decays from the point i according to the function f. When we force the Brownian bridge $\beta(s)$ for the potential $V^+_{\omega, u}$ to remain nearly the whole time t in the ball $K_{t^{1/\alpha}}$, we can govern the magnitude of the sum of the potential as follows: For each lattice point i "near" the starting point of the Brownian bridge you maximize f by M and force by restricting the domain of integration of E the respective ξ_i^+ to be small. For those points which are "far" away from the starting point of the Brownian bridge one maximizes ξ_i^+ by $\xi_{\max} - \xi_{\min}$. Then the magnitude of this part of the sum is determined by the decay of the function f.

The details follow in the next section.

4.2. Estimate for the Random Part

Lemma 7. There are two constants $c_5, c_6 > 0$ and a positive function $\varsigma(t)$ with

$$\lim_{t \to \infty} \frac{\ln \varsigma(t)}{t^\delta} = 0 \qquad \text{for all} \quad \delta > 0$$

such that

$$\tilde{A}^{\#}(t) \geqslant c_5 \varsigma(t)^{-c_6 t^{\nu/\alpha}} \int_{C_0} du \int_{5t^{1/\alpha} > |x| > 4t^{1/\alpha}} dx\, p(t, x)^2$$

$$\times \mathbb{E}_{0,0}^{t,x} \left[\exp\left(-\int_0^t V_{0,u}^{+}(\beta(s))\, ds \right) \chi_{\Omega_0(t^{1/\alpha})}(\beta) \right]$$

$$\times \mathbb{E}_{0,x}^{t,0} \left[\exp\left(-\int_0^t V_{0,u}^{-}(\beta'(s))\, ds \right) \chi_{\Omega_x'(t^{1/\alpha})}(\beta') \right] \tag{23}$$

where

$$\Omega_0(t^{1/\alpha}) = \{ \beta \mid |\beta(s)| < t^{1/\alpha} \text{ for all } 0 \leqslant s \leqslant t - t^{1/\alpha} \}$$

$$\Omega_x'(t^{1/\alpha}) = \{ \beta' \mid |\beta'(s) - x| < t^{1/\alpha} \text{ for all } 0 \leqslant s \leqslant t - t^{1/\alpha} \}$$

and

$$\chi_{\Omega_0(t^{1/\alpha})}(\beta), \chi_{\Omega_x'(t^{1/\alpha})}(\beta') = \begin{cases} 1, & \beta, \beta' \in \Omega_0(t^{1/\alpha}), \Omega_x'(t^{1/\alpha}) \\ 0, & \text{otherwise} \end{cases}$$

In the case of (18) $\varsigma(t)$ is a positive constant.

Proof. I. By restriction of the domain of integration we get

$$\tilde{A}^{\#}(t) \geqslant \int_{C_0} du \int_{5t^{1/\alpha} > |x| > 4t^{1/\alpha}} dx p(t, x)^2\, \mathbb{E}_{0,0}^{t,x} \otimes \mathbb{E}_{0,x}^{t,0} \Big[\chi_{\Omega_0(t^{1/\alpha})}(\beta)\, \chi_{\Omega_x'(t^{1/\alpha})}(\beta')$$

$$\times \exp\left(-\int_0^t V_{0,u}^{+}(\beta(s))\, ds \right) \exp\left(-\int_0^t V_{0,u}^{-}(\beta'(s))\, ds \right) \tag{24}$$

$$\times E\left(\exp\left(-\int_0^t \left(V_{\omega,u}^{+}(\beta(s)) + V_{\omega,u}^{-}(\beta'(s)) \right) ds \right) \right) \Big] \tag{25}$$

In the following steps we estimate (25) under consideration of the restricted domains of integration.

II. For the expectation value (25) we have indepent of the magnitude of $\beta(s)$ and $\beta'(s)$

$$(25) \geqslant e^{-t^{1/\alpha}(M^{+} + M^{-})} \underbrace{E\left(\exp\left(-\int_0^{t - t^{1/\alpha}} \left(V_{\omega,u}^{+}(\beta(s)) + V_{\omega,u}^{-}(\beta'(s)) \right) ds \right) \right)}_{=: (*)}$$

So it remains to estimate $(*)$ from below.

III. First from monotone convergence we know

$$\begin{aligned}
&\int_0^{t-t^{1/\alpha}} V^+_{\omega,u}(\beta(s))\,ds \\
&\quad=\int_0^{t-t^{1/\alpha}} \sum_{i\in\mathbb{Z}^\nu} \xi_i^+ f(\beta(s)+u-i)\,ds \\
&\quad= \sum_{i\in\mathbb{Z}^\nu,\,|i|<2t^{1/\alpha}} \xi_i^+ \int_0^{t-t^{1/\alpha}} f(\beta(s)+u-i)\,ds && (26)\\
&\qquad+\int_0^{t-t^{1/\alpha}} \sum_{i\in\mathbb{Z}^\nu,\,|i|\geqslant 2t^{1/\alpha}} \xi_i^+ f(\beta(s)+u-i)\,ds && (27)
\end{aligned}$$

and analogous for $\int_0^{t-t^{1/\alpha}} V^-_{\omega,u}(\beta'(s))\,ds$.

Observe that because of the restriction of the domain of integration over dx in I. The i with $|i|<2t^{1/\alpha}$ are all different to those with $|i-x|<2t^{1/\alpha}$. Thus the random variables ξ_i^+, ξ_i^- with these indices are independent and one has

$$\begin{aligned}
(*)\geqslant E\Bigg(\exp\Bigg(&-\sum_{i\in\mathbb{Z}^\nu,\,|i|<2t^{1/\alpha}} \xi_i^+(t-t^{1/\alpha})\,M \\
&-\sum_{i\in\mathbb{Z}^\nu,\,|i-x|<2t^{1/\alpha}} \xi_i^-(t-t^{1/\alpha})\,M\Bigg)\Bigg) && (28)\\
\times\exp\Bigg(&-(\xi_{\max}-\xi_{\min})\int_0^{t-t^{1/\alpha}} \sum_{i\in\mathbb{Z}^\nu,\,|i|\geqslant 2t^{1/\alpha}} f(\beta(s)+u-i)\,ds \\
&-(\xi_{\max}-\xi_{\min})\int_0^{t-t^{1/\alpha}} \sum_{i\in\mathbb{Z}^\nu,\,|i-x|\geqslant 2t^{1/\alpha}} f(\beta'(s)+u-i)\,ds\Bigg) && (29)
\end{aligned}$$

IV. In (28) we restrict the domain of integration of the expectation value E to the set

$$\left\{\xi_i^+<\frac{1}{t}\text{ for all }|i|<2t^{1/\alpha},\ \xi_i^-<\frac{1}{t}\text{ for all }|i-x|<2t^{1/\alpha}\right\}$$

This leads to

$$\begin{aligned}
(28)\geqslant&\exp\left(-2M\frac{t-t^{1/\alpha}}{t}\,2^\nu t^{\nu/\alpha}\right)\\
&\times P\{\xi_0-\xi_{\min}<1/t\}^{2^\nu t^{\nu/\alpha}}\,P\{\xi_{\max}-\xi_0<1/t\}^{2^\nu t^{\nu/\alpha}} && (30)
\end{aligned}$$

as the participated random variables are independent.

V. Now we estimate the first integral in (29) from above. Because of the assumptions

$$|\beta(s)| < t^{1/\alpha}, \qquad |i| \geqslant 2t^{1/\alpha}$$

one has

$$|\beta(s) + u - i| \geqslant |i| - |\beta(s)| - |u| \geqslant t^{1/\alpha} - \sqrt{v}$$

Therefore for t big enough there are constants $k_1, k_2, k_3, k_4 > 0$ depending only on the dimension with

$$\begin{aligned}
&\int_0^{t - t^{1/\alpha}} \sum_{i \in \mathbb{Z}^v,\, |i| \geqslant 2t^{1/\alpha}} f(\beta(s) + u - i)\, ds \\
&\quad \leqslant \gamma_2 \int_0^{t - t^{1/\alpha}} \sum_{i \in \mathbb{Z}^v,\, |i| \geqslant 2t^{1/\alpha}} |\beta(s) + u - i|^{-\alpha}\, ds \\
&\quad \leqslant \gamma_2 k_1 \int_0^{t - t^{1/\alpha}} \sum_{i \in \mathbb{Z}^v,\, = |i| \geqslant (1/2)\, t^{1/\alpha}} |i|^{-\alpha}\, ds \\
&\quad \leqslant \gamma_2 k_1 (t - t^{1/\alpha})\, k_2 \int_{|x| \geqslant k_3 t^{1/\alpha}} |x|^{-\alpha}\, dx \\
&\quad \leqslant k_4 t^{v/\alpha}
\end{aligned}$$

The estimate for the second integral is the same. We only need to replace $\beta(s)$ by $|\beta'(s) - x|$.

Summarized we get

$$(29) \geqslant e^{-2k_4 t^{v/\alpha}}. \quad \blacksquare$$

4.3. Estimate of the Determistic Rest of the Integral

In this subsection we show that the integral left behind in Lemma 7 has still the asymptotics sufficient for Theorem 5. Because of Proposition 6 we cannot expect to estimate by weaker asymptotics. Thus we have to estimate sharply. Therefore this problem is uncomparably more delicate than for the upper bound.

First we put the integral in a manageable form.

Lemma 8.

$$p(t,x)^2\, \mathbb{E}_{0,0}^{t,x}\left[\exp\left(-\int_0^t V_{0,u}^{+}(\beta(s))\,ds\right)\chi_{\Omega_0(t^{1/\alpha})}(\beta)\right]$$

$$\times\, \mathbb{E}_{0,x}^{t,0}\left[\exp\left(-\int_0^t V_{0,u}^{-}(\beta'(s))\,ds\right)\chi_{\Omega_x'(t^{1/\alpha})}(\beta')\right]$$

$$=\int_{|y|\leqslant t^{1/\alpha}} dy\; p(t-t^{1/\alpha},y)\, \mathbb{E}_{0,0}^{t-t^{1/\alpha},y}$$

$$\times\left[\exp\left(-\int_0^{t-t^{1/\alpha}} V_{0,u}^{+}(\beta(s))\,ds\right)\chi_{\Omega_0(t^{1/\alpha})}(\beta)\right]$$

$$\times\, p(t^{1/\alpha},x-y)\, \mathbb{E}_{0,y}^{t^{1/\alpha},x}\left[\exp\left(-\int_0^{t^{1/\alpha}} V_{0,u}^{+}(\beta(s))\,ds\right)\right]$$

$$\times\int_{|z-x|\leqslant t^{1/\alpha}} dz\; p(t-t^{1/\alpha},z-x)\, \mathbb{E}_{0,x}^{t-t^{1/\alpha},z}$$

$$\times\left[\exp\left(-\int_0^{t-t^{1/\alpha}} V_{0,u}^{-}(\beta'(s))\,ds\right)\chi_{\Omega_x'(t^{1/\alpha})}(\beta')\right]$$

$$\times\, p(t^{1/\alpha},z)\, \mathbb{E}_{0,z}^{t^{1/\alpha},0}\left[\exp\left(-\int_0^{t^{1/\alpha}} V_{0,u}^{-}(\beta'(s))\,ds\right)\right]$$

Proof. This is just an application of the Chapman–Kolmogoroff equalities.

As the Brownian bridges are continuous we get the domains of integration $\{y \mid |y|\leqslant t^{1/\alpha}\}$ respectively $\{z \mid |z-x|\leqslant t^{1/\alpha}\}$.

The Feynman–Kac-formula leads to

Lemma 9. There is a constant $c_7>0$, such that for t big enough and[5]

$$5t^{1/\alpha}>|x|>4t^{1/\alpha} \tag{31}$$

[5] The integration over dx in Lemma 7, (23) is just restricted to this set.

the expression in Lemma 8 is bigger or equal than

$$\exp(-c_7 t^{1/\alpha}) \tag{32}$$

$$\cdot \int_{|y| \leqslant t^{1/\alpha}} e^{-(t - t^{1/\alpha})(H_{0,u}^{+})_D^{t^{1/\alpha}}}(0, y)\, dy \tag{33}$$

$$\cdot \int_{|z - x| \leqslant t^{1/\alpha}} e^{-(t - t^{1/\alpha})(H_{0,u}^{-})_D^{t^{1/\alpha}}}(x, z)\, dz \tag{34}$$

With

$$e^{-(t - t^{1/\alpha})(H_{0,u}^{\pm})_D^{t^{1/\alpha}}}(\cdot, \cdot)$$

we denote the (continuous) kernels of the operators $e^{-(t - t^{1/\alpha})(H_{0,u}^{+})_D^{t^{1/\alpha}}}$. $(H_{0,u}^{\pm})_D^{t^{1/\alpha}}$ represent the operators $H_{0,u}^{-}$ respectively $H_{0,u}^{+}$ restricted to the balls

$$K_{t^{1/\alpha}} := \{ y \in \mathbb{R}^\nu \mid |y| < t^{1/\alpha} \}$$

respectively

$$K_{t^{1/\alpha}}(x) := \{ y \in \mathbb{R}\nu \mid |y - x| < t^{1/\alpha} \}$$

with Dirichlet boundary conditions.

Now to fulfil the proof of theorem 5, it suffices to estimate the integrals over the kernels (33) and (34) independent of x and u from below.

The first important step is

Proposition 10. Let V be a $\mathbb{Z}^\nu$-periodic potential with $V \leqslant \tilde{M}$, such that the Schrödinger operator

$$H = -\tfrac{1}{2}\Delta + V$$

has ground state zero. If H_D^{r, x_0} denotes its restriction to the ball

$$K_r(x_0) := \{ x \in \mathbb{R}^\nu \mid |x - x_0| < r \}$$

$x_0 \in \mathbb{R}^\nu$ with Dirichlet boundary conditions, then its spectrum is discrete. For its in L^2 normed groundstate eigenfunction denoted by ϕ_{r, x_0} belonging to the eigenvalue λ_{r, x_0} the following is valid:

1. It can be assumed to be continuous and this is assumed in the following.

2. It can be chosen strictly positive on the (open) ball $K_r(x_0)$ for all $r > 0$ and is assumed to be in the following.

3. It is under the assumptions 1 and 2 independent of x_0 and r, for r big enough, bounded from above by a constant

$$\eta = \eta(\tilde{M}) > 0$$

only depending on the dimension and $\tilde{M}$.

Proof. First we get by the Feynman–Kac formula the strict positivity, boundedness and continuity of the kernel of $e^{-sH_D^{r,x_0}}$.

Therefore $e^{-sH_D^{r,x_0}}$ maps functions in on continuous ones. By the spectral theorem 1 follows.

2 is an immediate consequence of Reed and Simon[9], Theorem XIII.44.

We are left to show 3. The following estimate is valid independent of x_0 and r.

Let h an arbitrary not negative function normed in L^2. Then by Simon[12] proof of Theorem B.1.1 we get

$$e^{-H_{0,u}^+} h(x) \leqslant k_1 \tag{35}$$

with some constant $k_1 > 0$ only depending on $\tilde{M}$. By the Feynman–Kac-formula one has

$$0 < e^{-H_D^{r,x_0}}(x, y) \leqslant e^{-H}(x, y) \qquad \text{for all} \quad x, y \in K_r(x_0)$$

and by the spectral theorem and (35) we get

$$\begin{aligned}\|e^{-\lambda_{r,x_0}}\phi_{r,x_0}\|_{L^\infty(K_r(x_0))} &= \|e^{-H_D^{r,x_0}}\phi_{r,x_0}\|_{L^\infty(K_r(x_0))}\\ &\leqslant \|e^{-H_{0,u}^+}\phi_{r,x_0}\|_{L^\infty(K_r(x_0))} \leqslant k_1\end{aligned}$$

In the next proposition 11 the velocity of convergence to zero of λ_{r,x_0} for $r \to \infty$ is shown. Hence the result. ∎

For the estimate of the eigenvalues λ_{r,x_0} we need

Proposition 11. Under the assumptions of proposition 10 there exists for given V a constant $c_8 > 0$ only depending on the dimension with

$$\lambda_{r,x_0} \leqslant c_8 r^{-2}$$

Proof. This follows by Kirsch/Simon[7] corollary to Proposition 5 and Reed/Simon[9], XIII.15. ∎

Now we are able to proceed in the estimate of the product of (33) and (34). We denote by

$$\varphi^+_{(t^{1/\alpha},\, u)},\ \varphi^-_{(t^{1/\alpha},\, u,\, x)}$$

the groundstate functions normed in L^2 of the operators $(H^+_{0,\,u})^{t^{1/\alpha}}_D$ respectively $(H^-_{0,\,u})^{t^{1/\alpha}}_D$ with belonging eigenvalues

$$\lambda^+_{(t^{1/\alpha},\, u)},\ \lambda^-_{(t^{1/\alpha},\, u,\, x)}$$

By Proposition 10, the spectral theorem and Propositon 11 we get

$$(33) \geqslant \frac{1}{\eta}\, e^{-(t - t^{1/\alpha})\, \lambda^+_{(t^{1/\alpha},\, u)}} \varphi^+_{(t^{1/\alpha},\, u)}(0) \geqslant \frac{1}{\eta}\, e^{-ktt^{-2/\alpha}} \varphi^+_{(t^{1/\alpha},\, u)}(0) \geqslant \frac{1}{\eta}\, e^{-kt^{\nu/\alpha}} \varphi^+_{(t^{1/\alpha},\, u)}(0) \tag{36}$$

Hence we just proved

Lemma 12. There are two constants $c_9, c_{10} > 0$ with

$$(33)(34) \geqslant c_9 e^{-c_{10} t^{\nu/\alpha}} \varphi^+_{(t^{1/\alpha},\, u)}(0)\, \varphi^-_{(t^{1/\alpha},\, u,\, x)}(x) \tag{37}$$

The last thing to show is that the eigenfunctions do not decay too fast to zero in the center of the ball of their domain.

Theorem 13. Let $H := -\frac{1}{2}\Delta + V$ be a Schrödinger operator with groundstate zero on $\mathbb{R}^\nu$. Assume V to be a $\mathbb{Z}^\nu$-periodic function, such that there exists a constant $\tilde{M}$ with $|V| \leqslant \tilde{M}$. Denote by H'^{r, x_0}_D the operator H restricted to the ball $K_r(x_0)$ with Dirichlet boundary conditions, so for its (continuous and positive) groundstate eigenfunction $\phi_{r,\, x_0}$ normed in L^2 in the center x_0 there is a positive constant c_{11} with

$$\phi_{r,\, x_0}(x_0) \geqslant e^{-c_{11} r^\nu} \tag{38}$$

for r big enough.

Proof. I. By combining the three theorems 3.3, 4.7 and 4.10 from Simader[10] we get[6] that for r big enough and R small enough there exists $n_0 \in \mathbb{N}$ independent of r and R with

$$|\phi_r(x_0) - \phi_r(x)| \leqslant \tfrac{1}{2}\phi_r(x_0) \tag{39}$$

for all $x_0 \in K_{(r-64R)}$ and $|x - x_0| \leqslant R/n_0$.

[6] Also for $\nu = 1$.

II. We want to determine a function $\varepsilon(r)$ such that

$$\int_{K_{r-\varepsilon(r)}} \phi_r^2(x)\,dx \geqslant \tfrac{1}{2} \tag{40}$$

Because of $\|\phi_r\|_{L^2(K_r)} = 1$ and Proposition 10, 3 we have

$$\int_{K_r \backslash K_{r-\varepsilon(r)}} \phi_r^2(x)\,dx \leqslant |K_r \backslash K_{r-\varepsilon(r)}|\,\eta^2(\tilde{M})$$

Thus for (40) it suffices to require

$$|K_r \backslash K_{r-\varepsilon(r)}|\,\eta^2(\tilde{M}) \leqslant \tfrac{1}{2} \tag{41}$$

As for some positive constant k_1 we get $|K_r \backslash K_{r-\varepsilon(r)}| \leqslant k_1 r^{\nu-1}\varepsilon(r)$ for r big enough we set

$$\varepsilon(r) = \frac{1}{2k_1\eta^2(\tilde{M})\,r^{\nu-1}} =: \frac{k_2}{r^{\nu-1}} \tag{42}$$

III. Define

$$R := \frac{\varepsilon(r)}{64} = \frac{k_2}{64r^{\nu-1}}$$

and

$$\rho := \frac{\varepsilon(r)}{64n_0} = \frac{R}{n_0}$$

Then for r big enough (39) is fulfilled for all $x_0 \in K_{r-\varepsilon(r)}$ and $|x - x_0| \leqslant \rho(r)$. It follows

$$|\phi_r(x) - \phi_r(x_0)| \leqslant \tfrac{1}{2}\phi_r(x_0) \Rightarrow \phi_r(x) \leqslant \tfrac{3}{2}\phi_r(x_0) \leqslant 3\phi_r(y)$$

That just means

$$\sup_{x \in K_{\rho(r)}(x_0)} \phi_r(x) \leqslant 3 \inf_{x \in K_{\rho(r)}(x_0)} \phi_r(x) \tag{43}$$

IV. As ϕ_r is continuous on K_r and the closure of $K_{r-\varepsilon(r)}$ denoted by $\overline{K_{r-\varepsilon(r)}}$ is compact, ϕ_r restricted to this closed set takes there its minimum and maximum. Denote these points in $\overline{K_{r-\varepsilon(r)}}$ by $x_{\min,r}$ respectively $x_{\max,r}$. Obviously we have

$$|x_{\max,r} - x_{\min,r}| \leqslant 2r$$

Therefore to cover the straight line from $x_{\max,r}$ to $x_{\min,r}$ by open balls $K_{\rho(r)}(x_i)$, such that $|x_i - x_{i-1}| \leqslant \rho(r)$, $x_i \in K_{r-\varepsilon(r)}$ for all i, $2r/\rho(r) = (128n_0/k_2)\, r^\nu$ balls are sufficient. Thus by (43)

$$\sup_{x \in K_{r-\varepsilon(r)}} \phi_r(x) \leqslant (3^{(128n_0/k_2)})^{r^\nu} \inf_{x \in K_{r-\varepsilon(r)}} \phi_r(x) =: k_3^{r^\nu} \inf_{x \in K_{r-\varepsilon(r)}} \phi_r(x) \tag{44}$$

V. The maximum of the function ϕ_r on $K_{r-\varepsilon(r)}$ is not smaller than the value of the constant function which satisfies (40). Thus

$$\sup_{x \in K_{r-\varepsilon(r)}} \phi_r(x) \geqslant \frac{1}{\sqrt{2\,|K_{r-\varepsilon(r)}|}} \geqslant \frac{1}{\sqrt{2\,|K_r|}} =: k_4 r^{-\nu/2}$$

Together with (44) this leads to

$$\phi_r(0) \geqslant \inf_{x \in K_{r-\varepsilon(r)}} \phi_r(x) \geqslant k_3^{-r^\nu} \sup_{x \in K_{r-\varepsilon(r)}} \phi_r(x) \geqslant k_4 r^{-\nu/2} k_3^{-r^\nu} \geqslant k_6^{-r^\nu}$$

and therefore to the assumption. ∎

With this Theorem 5 is completely proved.

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