Quantum evolution: The case of weak localization for a 3D alloy-type Anderson model and application to Hamiltonian based quantum computation

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(ABSTRACT)

Over the years, people have found Quantum Mechanics to be extremely useful in explaining various physical phenomena from a microscopic point of view. Anderson localization, named after physicist P. W. Anderson, states that disorder in a crystal can cause non-spreading of wave packets, which is one possible mechanism (at single electron level) to explain metal-insulator transitions. The theory of quantum computation promises to bring greater computational power over classical computers by making use of some special features of Quantum Mechanics. The first part of this dissertation considers a 3D alloy-type model, where the Hamiltonian is the sum of the finite difference Laplacian corresponding to free motion of an electron and a random potential generated by a sign-indefinite single-site potential. The result shows that localization occurs in the weak disorder regime, *i.e.*, when the coupling parameter λ is very small, for energies $E \leq -C\lambda^2$. The second part of this dissertation considers adiabatic quantum computing (AQC) algorithms for the unstructured search problem to the case when the number of marked items is unknown. In an ideal situation, an explicit quantum algorithm together with a counting subroutine are given that achieve the optimal Grover speedup over classical algorithms, *i.e.*, roughly speaking, reduce $O(2^n)$ to $O(2^{n/2})$, where n is the size of the problem. However, if one considers more realistic settings, the result shows this quantum speedup is achievable only under a very rigid control precision requirement (*e.g.*, exponentially small control error).

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Chapter 1

Introduction

1.1 Introduction to quantum mechanics, localization, and quantum computation

In classical mechanics, a particle is described by its position and momentum. It is understood that if there are some obstacles in the space, the particle simply cannot go through them and will bounce back if it hits those obstacles. But in quantum mechanics, a particle is described by the probability of it being in different positions, and a measurement will fix it at a certain position. This is the position representation of a quantum particle. The Fourier transform of the position representation conveniently transforms it to the momentum representation of the particle, where it is described by the probability of it being in different momentum states. One special feature of quantum mechanics is the uncertainty principle, which states that one cannot precisely measure both position and momentum of a particle at the same time. If one regards potential as the obstacles in classical mechanics, then one striking difference between classical mechanics and quantum mechanics is that in the quantum mechanical world, particles can tunnel through those "obstacles", meaning that there is possibility of locating a particle on the other side of those "obstacles", or even inside those "obstacles". Of course, if the potential is too strong, it will be difficult for a particle to travel through it. Then, one question is: in a random environment (meaning the potential is random), how will a particle behave? One intuitive answer is that if the energy of the particle is high enough, it can pass through all "obstacles". This corresponds to the so-called *extended states*. On the other hand, if the energy is low, then the particle will eventually die out (meaning the probability of locating it at infinity is 0 or arbitrarily small). This corresponds to the so called *localized states*. P. W. Anderson was the first to suggest electron localization inside a semiconductor, provided the degree of randomness of the impurities is large enough [7], and he won the Nobel prize for this in 1977. Ideally, one wants to show dynamical localization by solving the Schrödinger equation starting from a localized wave packet, or

investigating the higher moments of the system and its temporal dependence. But since the spectral localization will imply certain dynamical properties of the system (see Theorem 1.2.1 below), one can instead investigate the spectral properties of the system. This is often done in the literature and is also in this dissertation.

It turns out that there is a qualitative difference between the one-dimensional case and higher- dimensional cases. In a one-dimensional disordered system, the whole spectrum is pure point (eigenvalues). Since the Laplacian corresponds to free motion of particles and its spectrum is continuous, it means any disorder in the system completely destroys the transport property of the system. Thus, 'thin wires with impurities' should have low or even vanishing conductivity.

For dimensions $d \geq 3$, the situation is quite different. It's known that the spectrum consists of a union of closed intervals $\sum = \bigcup[a_i, b_i]$. When the disorder is small, localization occurs near the band edges. The spectrum well inside a band is believed to be absolutely continuous (though no rigorous proofs are given, except in the case where one restricts the structure of the underlying lattice to be a Cayley tree or something similar). The physical intuition is that there should be a phase transition from an insulating phase to a conducting phase. A transition point between these phases is called a *mobility edge*. On the other hand, when the disorder is large enough, localization occurs for the whole band $[a_i, b_i]$. So the qualitative picture is that initially, without any disorder in the system, the whole spectrum is absolutely continuous. As the disorder increases, the absolutely continuous spectrum is gradually eaten up by the pure point spectrum. Finally, when the disorder reaches a certain level, the whole spectrum becomes pure point. In this dissertation, we investigate the localization properties of a quantum system near the mobility edge when the disorder is extremely small, *i.e.*, the weak localization or lifshitz tails regime.

One special feature of quantum mechanics that is especially appealing to information science is the superposition of eigenstates, which lures one into thinking that a quantum system composed of qubits is able to store tremendously more information as compared with classical computers with ordinary bits, and the unitary evolution of those super-positioned states can actually solve classically difficult problems faster. It turns out that designing such quantum algorithms is extremely difficult, and there are only a few notable achievements. One is Grover's unstructured search [38], which is also the one considered in this dissertation. This is a problem for which one actually proves a quantum computer outperforms a classical computer. More specifically, it solves a problem with classical complexity $O(2^n)$ with time $O(2^{n/2})$, where n is the size of the problem. It is indeed an exponential speedup. Another one is Shor's algorithm for factoring large integers [66]. The asymptotic running time of Shor's algorithm is $O(b^3)$, where b is the number of digits of an integer, while the fastest classical algorithm known has order of growth roughly $O(\exp((Cb)^{1/3}))$, which is subexponential. The advent of Shor's algorithm greatly exhilarated theoretical computer scientists, because of the fact that integer factoring is believed to be outside of class P, and some even believed it to be NP-complete, albeit none of the above beliefs has been proven. In fact, proof of any of the above statements would be a major breakthrough. Apart from the difficulty in theoretically

determining the true power of a quantum computer, practical implementation of a quantum computer is also extremely difficult and it leads to proposals of different quantum computer models. Further introduction to this topic follows in Section 1.3.

1.2 Mathematical introduction to Anderson localization

In mathematics, we use functional spaces and operators acting on those spaces to describe quantum mechanics. It provides an intricate framework that have been used to explain the physical world exceedingly well, *e.g.*, many results derived from the most basic axioms has been tested by real world experiments. Here, a quantum mechanical particle moving in 3-dimensional space is described by a vector ψ in the Hilbert space $L^2(\mathbb{R}^3)$, called a wave function. $|\psi(x)|^2dx$ measures the probability of finding the particle between x and $x+dx$, and it satisfies the normalization condition $\int_{\mathbb{R}^3}|\psi(x)|^2dx = 1$. Besides position, a particle also has momentum, which in a quantum system is described by the Fourier transform of ψ,

$$\hat{\psi}(p) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\psi(x)e^{-ipx}dx.$$

The probability of finding a particle with momentum p is $|\hat{\psi}(p)|^2dp$. The time evolution of the wave function ψ is described by the Schrödinger equation:

$$i\frac{\partial}{\partial t}\psi = H\psi,$$

where $H = -\Delta + V$ is called the Hamiltonian. The operator Δ is the free Laplacian, corresponding to the kinetic part of the energy while V is the potential (a multiplication operator). It is easy to see that the evolution is unitary. We call E an energy of H if it belongs to $\sigma(H)$, the spectrum of H.

One common approximation used in physics literature is to allow the position space to be discrete, *i.e.* $\mathbb{Z}^3$. Then, the corresponding Hilbert space for the wave function is $l^2(\mathbb{Z}^3)$. The Hamiltonian H is also modified and Δ becomes a finite difference Laplacian:

$$(\Delta\psi)(x) \;=\; \sum_{e\in\mathbb{Z}^3,\ |e|=1} \psi(x+e) \;-\; 6\psi(x)\,. \tag{1.1}$$

One can further restrict the system to a bounded region on $\mathbb{Z}^3$. This will make the Hamiltonian finite dimensional; *i.e.*, a finite dimensional matrix.

Now, consider an electron moving in a crystal, where we think of the crystal as a periodic lattice $\mathbb{Z}^3$. Atoms or nuclei reside on lattice sites. The electron feels a potential of the form

$qu(x-i)$ at point $x \in \mathbb{Z}^3$ due to an atom with charge q (*e.g.*, an ion) located at the point $i \in \mathbb{Z}^3$. So in a regular crystal, the particle is exposed to a total potential:

$$V(x) = \sum_{i \in \mathbb{Z}^3} qu(x-i).$$

The force between the atom at position i and the electron at position x is measured by the potential. The Anderson alloy-type model puts q to be a random quantity, with the rationale that when several materials are mixed together, there is variability in q at a particular lattice point. Several common types of distribution for q have become the target of intensive research, though the common Bernoulli distribution in the discrete setting poses an extremely difficult problem and is still open. The Bernoulli distribution in the continuous setting was solved by J. Bourgain and C. Kenig [13]. Some assumptions on the probability density functions are needed in order to have meaningful results.

Assumption 1. Charge q at position i has probability measure P_0 with compactly supported and bounded density ρ.

From now on, I will switch notation and use $w(i)$ to denote q at position $i \in \mathbb{Z}^3$. The potential then becomes:

$$V_\omega(x) = \sum_{i \in \mathbb{Z}^3} \lambda \omega(i) u(x-i), \;\; x \in \mathbb{Z}^3, \tag{1.2}$$

where λ is the strength of the disorder. This dissertation concerns the regime where λ is very small, the so called weak disorder regime.

It is well known in functional analysis that the spectrum of any self-adjoint operator H on a Hilbert space $\mathcal{H}$ consists of a pure point part $\sigma_{pp}(H)$, an absolutely continuous part $\sigma_{ac}(H)$ and a singular continuous part $\sigma_{sc}(H)$. The spectral property of an energy is important in the study of a quantum system, as manifested by the following theorem [21].

Theorem 1.2.1. *Let Λ_L denote a cube in $\mathbb{Z}^d$ centered at the origin with side length $L+1$. Then*

$$\lim_{L \to \infty} \sup_t \sum_{x \notin \Lambda_L} \langle \delta_x, e^{-itH} P_{pp}(H) \psi \rangle^2 = 0$$

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \sum_{x \in \Lambda} \langle \delta_x, e^{-itH} P_c(H) \psi \rangle^2 dt = 0$$

where P_{pp} and P_c are projections onto the spaces associated with $\sigma_{pp}(H)$ and $\sigma_c(H)$ respectively.

In a first approximation to Equ. (1.2), $u(x-i) = \delta_x(i)$, the effect is that all atoms, except the one at the same position as the electron, are ignored. So,

$$V_\omega(x) = \lambda \omega(x), \;\; x \in \mathbb{Z}^3, \;\; \omega(x) \text{ has probability measure } P_0. \tag{1.3}$$

Let $e(p)$ denote the dispersion law, associated with the Fourier transform of the Laplacian, $(\mathcal{F}\Delta f)(p) = -2e(p)\hat{f}(p)$, where

$$\hat{f}(p) := (\mathcal{F}f)(p) := \sum_{n\in\mathbb{Z}^3} e^{-i2\pi p\cdot n} f(n)\,, \quad p \in \mathbb{T}^3 := [-1/2, 1/2]^3\,,$$

An easy calculation shows

$$e(p) = 2\sum_{\alpha=1}^{3} \sin^2(\pi p \cdot e_\alpha)\,, \tag{1.4}$$

where e_α is a unit vector in the α direction. So the spectrum of $-\Delta$ is absolutely continuous and consists of the interval $[0, 12]$. On the other hand, the spectrum of V_ω is of the pure point type and $\sigma(V_\omega) = \text{supp}\rho$ for P-almost all ω, where ρ is the probability density function of ω, with eigenfunctions $\delta_i(x)$. Then the question is: What is the spectrum of the Hamiltonian $H_\omega = -\Delta + V_\omega$?

In order to answer this question, we introduce the notion of ergodicity: Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. A measurable mapping $T : \Omega \to \Omega$ is called a probability preserving transformation if $\mathbb{P}(T^{-1}E) = \mathbb{P}(E)$ for every $E \in \mathcal{F}$. T is called ergodic if for every $E \in \mathcal{F}$ such that $T^{-1}E = E$, $\mathbb{P}(E)$ is either 0 or 1. Those E's are called invariant sets.

Theorem 1.2.2 (Birkhoff[52])**.** *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, and T a probability preserving transformation. If $f \in L^1$, then $\lim_{N\to\infty} \frac{1}{N}\sum_{k=0}^{N-1} f \circ T^k$ exists $\mathbb{P}$-a.e. and is T-invariant. If further T is ergodic, then the limit is $\int f d\mathbb{P}$.*

Remark 1. If we define $X_i = f \circ T^i$, then $\{X_i\}_{i\in\mathbb{Z}^+}$ is a stochastic process, and the above theorem says $\lim_{N\to\infty} \frac{1}{N}\sum_{k=0}^{N-1} X_i \to \mathbb{E}(X_0)$. This generalizes naturally to stochastic processes indexed by $\mathbb{Z}^d$.

Let $\{T_i\}_{i\in\mathbb{Z}^d}$ be a family of measure preserving transformations on $\Omega = \mathbb{R}^{\mathbb{Z}^d}$. $E \in \mathcal{F}$ is called invariant under $\{T_i\}_{i\in\mathbb{Z}^d}$ if $T_i^{-1}E = E$ for all $i \in \mathbb{Z}^d$. Then $\{T_i\}_{i\in\mathbb{Z}^d}$ is called ergodic if any invariant E has probability 0 or 1. A stochastic process $\{X_i\}_{i\in\mathbb{Z}^d}$ is called ergodic if there exists an ergodic family of measure preserving transformations $\{T_i\}_{i\in\mathbb{Z}^d}$ such that $X_i(T_j\omega) = X_{i-j}(\omega)$.

Theorem 1.2.3. *If $\{X_i\}_{i\in\mathbb{Z}^d}$ is an ergodic process on $(\Omega, \mathcal{F}, \mathbb{P})$ and $\mathbb{E}(|X_0|) < \infty$ then*

$$\lim_{L\to\infty} \frac{1}{(L+1)^d} \sum_{i\in\Lambda_L} X_i = \mathbb{E}(X_0)$$

for $\mathbb{P}$-almost all ω.

As one can verify, the random potential $V_\omega(x), x \in \mathbb{Z}^3$ is an ergodic process with $\{T_i\}_{i\in\mathbb{Z}^3}$ being all the translations on $\mathbb{Z}^3$.

Define translation operators $\{U_i\}_{i\in\mathbb{Z}^d}$ on $\ell^2(\mathbb{Z}^d)$ by $(U_i\psi)_m = \psi_{m-i}$. Then the operators U_i are unitary, and the multiplication operator V_ω satisfies $V_{T_i\omega} = U_i V_\omega U_i^*$. The free Laplacian Δ commutes with U_i. Thus

$$H_{T_i\omega} = U_i H_\omega U_i^*. \tag{1.5}$$

Operators satisfying (1.5) (with ergodic T_i and unitary U_i) are called ergodic operators.

A useful result for unitary operators is

Lemma 1.2.4. *Let A be a self adjoint operator and U a unitary operator, then for any bounded measurable function f*

$$f(UAU^*) = Uf(A)U^*$$

The following result due to Pastur [45] shows that the spectrum of H_ω is a constant set for $\mathbb{P}$-almost all ω.

Theorem 1.2.5 (Pastur)**.** *If H_ω is an ergodic family of selfadjoint operators, then there is a closed, nonrandom subset Σ of $\mathbb{R}$, such that*
$\sigma(H_\omega) = \Sigma$ for $\mathbb{P}$-almost all ω
Moreover, there are sets Σ_{ac}, Σ_{sc} and Σ_{pp} such that
$\sigma_{ac}(H_\omega) = \Sigma_{ac}$, $\sigma_{sc}(H_\omega) = \Sigma_{sc}$, $\sigma_{pp}(H_\omega) = \Sigma_{pp}$ for $\mathbb{P}$-almost all ω.

Proof. If H_ω is ergodic and f is a bounded measurable function, then by Equ. (1.5) and Lemma 1.2.4,

$$f(H_{T_i\omega}) = f(U_i H_\omega U_i^*) = U_i f(H_\omega) U_i^*.$$

Thus, $f(H_\omega)$ is ergodic, too. In particular, $\chi_{(\lambda,\mu)}(H_\omega)$ is ergodic.

$(\lambda,\mu)\cap\sigma(H_\omega) \neq \emptyset$ if and only if $\chi_{(\lambda,\mu)}(H_\omega) \neq 0$ if and only if $\operatorname{Tr}\chi_{(\lambda,\mu)}(H_\omega) \neq 0$. Let $X_i = \langle\delta_i, \chi_{(\lambda,\mu)}(H_\omega)\delta_i\rangle$, then $\{X_i\}_{i\in\mathbb{Z}^d}$ is a ergodic process (see Proposition 1.2.7 below). By ergodic theorem 1.2.3, $\operatorname{Tr}\chi_{(\lambda,\mu)}(H_\omega) = \sum_{i\in\mathbb{Z}^d} X_i = c_{\lambda,\mu}$ for all $\omega\in\Omega_{\lambda,\mu}$ with $\mathbb{P}(\Omega_{\lambda,\mu}) = 1$. Set

$$\Sigma = \{E | c_{\lambda,\mu} \neq 0 \text{ for all } \lambda < E < \mu, \quad \lambda,\mu\in\mathbb{Q}\},$$

then $\sigma(H_\omega) = \Sigma$ for $\omega\in\Omega_0$, where

$$\Omega_0 = \bigcap_{\lambda,\mu\in\mathbb{Q}, c_{\lambda,\mu}\neq 0} \Omega_{\lambda,\mu}.$$

Since Ω_0 is a countable intersection of sets of full measure, $\mathbb{P}(\Omega_0) = 1$. The same conclusion holds for σ_{ac} if the projection onto $\mathcal{H}_{ac}$ is measurable. Similar for σ_{sc} and σ_{pp}. See [19] for proof of measurability. □

Also it is shown that

Theorem 1.2.6. *For $\mathbb{P}$-almost all ω we have $\sigma(H_\omega) = [0, 4d] + \operatorname{supp}\rho$.*

Proof. We already know by using Fourier transform that $\sigma(-\Delta) = [0, 4d]$. $\sigma(V_\omega) = \text{supp}\rho$ for $\mathbb{P}$-almost all ω with eigenfunctions $\delta_i(x)$. Now for any self-adjoint operator A, a bounded self-adjoint operator B, the Neumann series for $(A + B - E)^{-1}$ is

$$\frac{1}{A+B-E} = \frac{1}{A-E}\sum_{i=1}^{\infty}\left(B\frac{1}{A-E}\right)^i$$

the series is convergent for $E \notin \sigma(A)$ and $\text{dist}(E, \sigma(A)) > \|B\|$. Thus, $\sigma(A + B) \subset \sigma(A) + [-\|B\|, \|B\|]$. Now set $A = V_\omega$ and $B = -\Delta - 2d$, we get $\|B\| = 2d$ and in turn $\sigma(-\Delta - 2d + V_\omega) \subset \sigma(V_\omega) + [-2d, 2d]$. This shows $\sigma(-\Delta + V_\omega) \subset \sigma(V_\omega) + [0, 4d]$.

In order to prove the converse, we will utilize the following Weyl Criterion (see [64]):

$$\lambda \in \sigma(H_\omega) \quad \Leftrightarrow \quad \exists\, \psi_n \in D_0 \text{ with } \|\psi_n\| = 1 : \|(H_\omega - \lambda)\psi_n\| \to 0,$$

where D_0 is any vector space such that H_ω is essentially self-adjoint on D_0. The sequence ψ_n is called a Weyl sequence.

Now, pick a countable and dense subset $S_0 \subset \text{supp}\rho$. $\forall \lambda_1 \in S_0$, $\exists \Omega_{\lambda_1} \subset \Omega$ s.t. $\mathbb{P}(\Omega_{\lambda_1}) = 1$, and $\lambda_1 \in \sigma(V_\omega)$, $\forall \omega \in \Omega_{\lambda_1}$. Let $\lambda_0 \in \sigma(-\Delta)$, and $\lambda = \lambda_0 + \lambda_1$. we'll construct a Weyl sequence for λ by taking $D_0 = \ell_0^2(\mathbb{Z}^d)$. First let ϕ_n be a Weyl sequence for $-\Delta$ and λ_0, *i.e.*, $\|(-\Delta - \lambda_0)\phi_n\| < 1/n$, $\phi_n \in D_0$ and $\|\phi_n\| = 1$. If we set $\phi^{(j)}$ to be a translation of ϕ, *i.e.*, $\phi^{(j)}(i) = \phi(i - j)$, then we still have $H_0\phi^{(j)} = (H_0\phi)^{(j)}$. Now for any ϕ_n, we can find a sequence $\{j_n^m\}_{m=1}^{\infty}$, $\|j_n^m\| \to \infty$ such that

$$\sup_{i \in \text{supp}\phi_n} |V_\omega(i + j_n^m) - \lambda_1| < \frac{1}{m}.$$

Finally define $\psi_n = \phi_n^{(j_n^n)}$. ψ_n is our desired Weyl sequence. So $\lambda \in \sigma(H_\omega)\, \forall \omega \in \Omega_{\lambda_1}$. Let $\tilde{\Omega} := \bigcap_{\lambda_1 \in S_0} \Omega_{\lambda_1}$, then $\mathbb{P}(\tilde{\Omega}) = 1$. Moreover, $[0, 4d] + S_0 \subset \sigma(H_\omega)\, \forall \omega \in \tilde{\Omega}$. Since $\sigma(H_\omega)$ is a closed set with probability 1 by Theorem 1.2.5, we get $[0, 4d] + \text{supp}\rho \subset \sigma(H_\omega)$. □

Anderson localization is a statement that under certain conditions, Σ_{pp} in Theorem 1.2.5 is nonempty. By far, localization is well understood under the assumption $u(x - i) = \delta_x(i)$.

In the case $d = 1$, Anderson localization exists for all energies for a huge class of randomness. In the case $d = 3$, Anderson localization has been proven at low energies and high disorder when the underlying probability measure assumes some regularity condition, for example, the existence of a bounded probability density. The proof of localization for 3-d models uses either the so called multiscale analysis (MSA) or fractional moment method. [47] contains an accessible introduction to MSA while [68] explains the fractional moment method.

One important quantity for a random Schrödinger operator is the density of states. The density of states measure $\nu([E_1, E_2])$ measures the number of states per unit volume with energy between E_1 and E_2.

Let's begin with some definitions. By $\Lambda_L(x)$ we mean the cube centered at x with sides of length L, so $\Lambda_L(x) = \{y \in \mathbb{Z}^d; \|y - x\|_\infty \leq L/2\}$. $\partial\Lambda_L(x)$ denotes its boundary, *i.e.*:

$$\partial\Lambda_L(x) = \left\{ \langle y, y' \rangle; y \in \Lambda_L(x), y' \notin \Lambda_L(x), \sum_{i=1}^{d} |y_i - y'_i| = 1 \right\}.$$

The inner boundary of $\Lambda_L(x)$ is defined by:

$$\partial\Lambda_L^-(x) = \{y \in \mathbb{Z}^d; \langle y, y' \rangle \in \partial\Lambda_L(x) \text{ for some } y' \notin \Lambda_L(x)\}.$$

Similarly the outer boundary is defined by:

$$\partial\Lambda_L^+(x) = \{y' \in \mathbb{Z}^d; \langle y, y' \rangle \in \partial\Lambda_L(x) \text{ for some } y \in \Lambda_L(x)\}.$$

We have;

$$|\Lambda_L(x)| \leq (L+1)^d, \quad |\partial\Lambda_L(x)| \leq s_d(L+1)^{d-1}$$

where s_d is a constant that only depends on dimension d.

Now, define the following quantity

$$\nu_L(\psi) = \frac{1}{|\Lambda_L|} \operatorname{Tr}(\chi_{\Lambda_L} \psi(H_\omega) \chi_{\Lambda_L}) = \frac{1}{|\Lambda_L|} \operatorname{Tr}(\psi(H_\omega) \chi_{\Lambda_L}),$$

where χ_{Λ_L} is the characteristic function on Λ_L. Since ν_L is a positive linear functional on the bounded continuous functions, by the Riesz representation theorem, it corresponds to a measure which we also denote by ν_L,

$$\nu_L(\psi) = \int_{\mathbb{R}} \psi(\lambda) d\nu_L(\lambda).$$

Proposition 1.2.7. *If ψ is a bounded measurable function, then for $\mathbb{P}$-almost all ω*

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \operatorname{Tr}(\psi(H_\omega)\chi_{\Lambda_L}) = \mathbb{E}(\langle \delta_0, \psi(H_\omega)\delta_0 \rangle)$$

Proof.

$$\frac{1}{|\Lambda_L|} \operatorname{Tr}(\psi(H_\omega)\chi_{\Lambda_L}) = \frac{1}{(L+1)^d} \sum_{i \in \Lambda_L} \langle \delta_i, \psi(H_\omega)\delta_i \rangle.$$

Define $X_i = \langle \delta_i, \psi(H_\omega)\delta_i \rangle$. Since shift operators $\{T_i\}$ are ergodic and

$$\begin{aligned} X_i(T_j\omega) &= \langle \delta_i, \psi(H_{T_j\omega})\delta_i \rangle \\ &= \langle \delta_i, \psi(U_i H_\omega U_i^*)\delta_i \rangle \\ &= \langle \delta_i, U_i \psi(H_\omega) U_i^* \delta_i \rangle \\ &= \langle U_i^* \delta_i, \psi(H_\omega) U_i^* \delta_i \rangle \\ &= \langle \delta_{i-j}, \psi(H_\omega)\delta_{i-j} \rangle \\ &= X_{i-j}(\omega), \end{aligned}$$

$\{X_i\}_{i\in\mathbb{Z}^d}$ is an ergodic process. Also we have $\mathbb{E}(|X_i|) \le \|\psi\|_\infty$. Thus, by the ergodic theorem 1.2.3,

$$\frac{1}{|\Lambda_L|}\operatorname{Tr}(\psi(H_\omega)\chi_{\Lambda_L}) = \frac{1}{(L+1)^d}\sum_{i\in\Lambda_L} X_i \;\to\; \mathbb{E}(X_0) = \mathbb{E}(\langle\delta_0, \psi(H_\omega)\delta_0\rangle)$$

as $L\to\infty$. □

Now we are able to define the density of states measure. For any Borel set A in $\mathbb{R}$,

$$\nu(A) = \mathbb{E}(\langle\delta_0, \chi_A(H_\omega)\delta_0\rangle). \tag{1.6}$$

The integrated density of states is then defined by

$$N(E) = \nu((-\infty, E]). \tag{1.7}$$

In fact, one can show that ν_L converges vaguely to ν $\mathbb{P}$-almost surely as $L\to\infty$.

An alternative approach to the density of states is first define the measure $\tilde{\nu}_L$ by

$$\int \psi(\lambda)d\tilde{\nu}_L(\lambda) = \frac{1}{|\Lambda_L|}\operatorname{Tr}\psi(H_{\Lambda_L}).$$

where H_Λ is the restriction of H_ω to $\Lambda\subset\mathbb{Z}^3$. It is defined by $H_\Lambda(n,m) = \langle\delta_n, H_\omega\delta_m\rangle$ whenever both n and m belong to Λ. Define $E_n(H_\Lambda)$ to be the nth eigenvalue of H_Λ, *i.e.*, $E_1 < E_2 < \cdots < E_n < \cdots < E_{|\Lambda|}$. Then since $\psi(H_{\Lambda_L})$ is a finite matrix, it amounts to

$$\int \psi(\lambda)d\tilde{\nu}_L(\lambda) = \frac{1}{|\Lambda_L|}\sum_n \psi(E_n(H_{\Lambda_L}).$$

Now we define the eigenvalue counting function

$$N_\Lambda(E) = |\{n|E_n(H_\Lambda) < E\}|.$$

With this notation,

$$\frac{1}{|\Lambda_L|}N_\Lambda(E) = \int \chi_{(-\infty,E)}(\lambda)d\tilde{\nu}_L(\lambda).$$

Again, it can be shown that $\tilde{\nu}_L$ converges vaguely to ν_L $\mathbb{P}$-almost surely.

The Wegner estimate establishes the regularity of the density of states.

Theorem 1.2.8 (Wegner)**.** *Suppose the measure P_0 for the potential in Equ.* (1.3) *has a bounded density g, then*

$$\mathbb{E}(N_\Lambda(E+\epsilon) - N_\Lambda(E-\epsilon)) \le C\,\|g\|_\infty\,\epsilon\,|\Lambda|$$

There are two important corollaries that follow from the above theorem.

Corollary 1.2.9. *Under the assumption of 1.2.8 the integrated density of states is absolutely continuous with a bounded density $n(E)$.*

Proof. Since for $\mathbb{P}$-almost all ω

$$\frac{1}{|\Lambda|}N_\Lambda(E) \to N(E),$$

we have

$$N(E+\epsilon) - N(E-\epsilon) = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|}\mathbb{E}(N_\Lambda(E+\epsilon) - N_\Lambda(E-\epsilon)) \leq C \left\|g\right\|_\infty \epsilon$$

Thus, there exists $n(E)$ such that $N(E) = \int_{-\infty}^{E} n(\lambda)d\lambda$. □

Remark 2. We call $n(E)$ the density of states.

Corollary 1.2.10. *Under the assumption of 1.2.8 we have for any E and Λ*

$$\mathbb{P}(\mathrm{dist}(E, \sigma(H_\Lambda)) < \epsilon) \leq C \left\|g\right\|_\infty \epsilon \left|\Lambda\right|$$

Proof. By the Chebycheff inequality we get

$$\begin{aligned} \mathbb{P}(\mathrm{dist}(E, \sigma(H_\Lambda)) < \epsilon) &= \mathbb{P}(N_\Lambda(E+\epsilon) - N_\Lambda(E-\epsilon)) \\ &\leq \mathbb{E}(N_\Lambda(E+\epsilon) - N_\Lambda(E+\epsilon)) \\ &\leq C \left\|g\right\|_\infty \epsilon \left|\Lambda\right|. \end{aligned}$$

□

The Wegner estimate, especially the conclusion of Corollary 1.2.10 is a key ingredient to MSA.

Another quantity of interest in the proof of localization is the so called Green's function. It is defined by $R_\Lambda(E) = (H_\Lambda - z)^{-1}$ for $E \notin \sigma(H_\Lambda)$. We write

$$G_\Lambda(E; x, y) = (H_\Lambda - E)^{-1}(x, y) \quad \text{for} \quad x, y \in \Lambda.$$

If $\Lambda = \mathbb{Z}^d$ then we simply write $G(E; x, y)$.

Definition. Let $m > 0$, $E \in R$. A cube $\Lambda_L(x)$ is (m, E)-regular (for a fixed potential) if $E \notin \sigma(H_{\Lambda_L(x)})$ and

$$\left|G_{\Lambda_L(x)}(E; x, y)\right| \leq e^{-mL} \quad \text{for all} \quad y \in \partial\Lambda_L(x).$$

Otherwise we say that $\Lambda_L(x)$ is (m, E)-singular.

We say $\psi \in \ell^2(\mathbb{Z}^d)$ decays exponentially fast with mass m if there exists a constant m such that

$$\limsup_{\|x\|\to\infty} \frac{\log|\psi(x)|}{\|x\|} \leq -m$$

The following MSA for proving localization is due to Von Dreifus and Klein [24].

Theorem 1.2.11. *Let $E_0 \in R$. Suppose that, for some $L_0 > 0$, we have:*

(C1) $\mathbb{P}\{\Lambda_{L_0}(0) \text{ is } (m_0, E_0)-\text{regular}\} \geq 1 - 1/L_0^p$ *for some $p > d$, $m_0 > 0$.*

(C2) $\mathbb{P}\{d(E, \sigma(H_{\Lambda_L(0)})) < e^{-L^\beta}\} \leq 1/L^q$ *for some β and q, $0 < \beta < 1$, $q > 4p + 6d$, all E with $|E - E_0| \leq \eta$, where $\eta > 0$, and all $L \geq L_0$.*

Then, given m, $0 < m < m_0$, there exists $B = B(p, d, \beta, q, m_0, m) < \infty$, such that if $L_0 > B$, we can find $\delta = \delta(L_0, m_0, m, \beta, \eta) > 0$, so, with probability one, the spectrum of H in $(E_0 - \delta, E_0 + \delta)$ is pure point and the eigenfunctions corresponding to eigenvalues in $(E_0 - \delta, E_0 + \delta)$ decay exponentially fast at infinity.

Notice if $d(E, \sigma(H_{\Lambda_L(0)})) \geq e^{-L_0^\beta}$ and $|E - E_0| \leq \frac{1}{2}e^{-L_0^\beta}$, we have that $d(E, \sigma(H_{\Lambda_{L_0}(0)})) \geq \frac{1}{2}e^{-L_0^\beta}$. If $\Lambda_{L_0(0)}$ is (m_0, E_0)-regular and $y \in \partial\Lambda_{L_0}(0)$, then the resolvent equation

$$G_{\Lambda_{L_0}(0)}(E) = G_{\Lambda_{L_0}(0)}(E_0) + (E - E_0)G_{\Lambda_{L_0}(0)}(E)G_{\Lambda_{L_0}(0)}(E_0)$$

implies

$$\left|G_{\Lambda_{L_0}(0)}(E; 0, y)\right| \leq e^{-m_0 L_0} + 2\,|E - E_0|\, e^{2L_0^\beta}.$$

Then $G_{\Lambda_{L_0}(0)}$ is (m_0', E)-regular if $|E - E_0| \leq \delta = \frac{1}{2}e^{-2L_0^\beta}(e^{-m_0' L_0} - e^{-m_0 L_0})$. So

$$\begin{aligned}
& \mathbb{P}\big\{\forall E \in (E_0 - \delta, E_0 + \delta) \quad \Lambda_{L_0}(0) \text{ is } (m_0', E)-\text{regular}\big\} \\
= \;& \mathbb{P}\big\{\Lambda_{L_0}(0) \text{ is } (m_0, E_0)-\text{regular} \;\cap\; d(E, \sigma(H_{\Lambda_L(0)})) < e^{-L^\beta}\big\} \\
\geq \;& 1 - \frac{1}{L_0^p} - \frac{1}{L_0^q} \\
\geq \;& 1 - \frac{1}{L_0^{p'}}
\end{aligned}$$

where m_0' and p' are chosen that $0 < m_0' < m_0$ and $d < p' < p$. How large one needs to choose L_0 here depends on p, q and p'. Because of independence of the cubes, it follows $\mathbb{P}\{\forall E \in I$ either $\Lambda_{L_0}(x)$ or $\Lambda_{L_0}(y)$ is $(m_0, E)-\text{regular}\} \geq 1 - 1/L_0^{2p}$ for some $p > d$, $m_0 > 0$, and any $x, y \in \mathbb{Z}^d$ with $\|x - y\| > L_0$.

The proof consists of two components. One is an inductive process that establishes the following statement for a sequence of $L_{k+1} = L_k^\alpha$, $k = 0, 1, 2, \ldots$, where $1 < \alpha < 2$ and $0 < m < m_0$:

$$\mathbb{P}\big\{\forall E \in I \text{ either } \Lambda_{L_k}(x) \text{ or } \Lambda_{L_k}(y) \text{ is } (m, E)-\text{regular}\big\} \geq 1 - 1/L_k^{2p} \tag{1.8}$$

for any $x, y \in \mathbb{Z}^d$ with $\|x - y\| > L_0$.

The second component establishes exponential decay of eigenfunctions with mass m corresponding to eigenvalues in I. The idea is to show that the generalized eigenfunctions corresponding to $E \in I$, which a priori only have a polynomial bound at infinity, in fact decay exponentially fast given the above condition (1.8). See [24] for details.

Next, we establish the initial volume estimate and thus prove localization for large disorder. The bound on the probability density g of a random variable $\omega(i)$, $\|g\|_\infty$, is a measure of the disorder. The smaller $\|g\|_\infty$ is, the wider the random variable spreads.

Theorem 1.2.12. *Suppose the distribution P_0 has a bounded density g. Then for any E, L_0 and $m_0 > 0$, there is a $\rho > 0$ such that when $\|g\|_\infty < \rho$,*

$$\mathbb{P}\{\Lambda_{L_0}(0) \text{ is not } (m_0, E)-\text{regular}\} \leq 1/L_0^p$$

Proof. Since $\left|G_{\Lambda_{L_0}(0)}(E; 0, x)\right| \leq \left\|(H_{\Lambda_{L_0}(0)} - E)^{-1}\right\|$ we have

$$\begin{aligned}
& \mathbb{P}\left[\left|G_{\Lambda_{L_0}(0)}(E; 0, x)\right| > e^{-m_0 L_0}\right] \\
\leq\ & \mathbb{P}\left[\left\|(H_{\Lambda_{L_0}(0)} - E)^{-1}\right\| > e^{-m_0 L_0}\right] \\
\leq\ & \mathbb{P}\big[\operatorname{dist}(E, \sigma(H_{\Lambda_{L_0}(0)})) < e^{m_0 L_0}\big] \\
\leq\ & C \|g\|_\infty e^{m_0 L_0} |\Lambda_{L_0}(0)|
\end{aligned}$$

where in the last step we used Corollary 1.2.10. Now we can choose ρ small enough so that we get the desired estimate. □

As discussed in Section 1.1, it is of great interest to the physics community to find the quantitative boundary (if it exists) that separates Σ_{pp} and Σ_{ac} for 3-d Anderson model, because it indicates that a phase transition exists from an insulating phase to a conducting phase. In the Lifshitz regime, several works intend to quantify the localization region at the bottom of the spectrum, *i.e.*, to establish a lower bound E_0 such that localization occurs for $E < E_0$. The spectrum starts from $-C\lambda$, where $-C = \inf \rho$. Let us mention the work of M. Aizenman [2] that established localization below $E_0(\lambda) = -C\lambda + O(\lambda^{5/4})$, the improvement by W-M. Wang [70] to $E_0(\lambda) = -C\lambda + O(\lambda)$, by F. Klopp [51] to $E_0(\lambda) = -\tilde{C}\lambda^{7/6}$, with $\tilde{C} > 0$, and the predecessor of this dissertation work by A. Elgart that established $E_0(\lambda) = -\hat{C}\lambda^2$, with $\hat{C} > 0$, following the unpublished note of T. Spencer [67].

This dissertation assumes the more realistic assumption that u is an exponentially decaying function. The result is, roughly speaking, localization still occurs for $E < E_0(\lambda) = \hat{C}\lambda^2$ with $\hat{C} < 0$. The proof uses MSA. There are two issues one needs to verify before proceeding. The first is that $\sigma(H_\omega)$, $\sigma_{pp}(H_\omega)$, $\sigma_{ac}(H_\omega)$ and $\sigma_{sc}(H_\omega)$ are still fixed sets with probability one. This is true due to the ergodicity of H_ω, *e.g.*, the proof of Theorem 1.2.5 goes through without much modification. The second is the generalization of MSA to the case of u being an exponentially decaying function. This is addressed by Kirsch, Stollmann and Stolz in [48]. Finally, some proofs presented in this dissertation can also be found in [17].

1.3 Introducing adiabatic quantum computation

As introduced in Section 1.1, quantum computing is believed to possess more computational power than classical computing on certain computational tasks. The basic paradigm, which is usually used in the theoretical works on quantum computing, is the so called quantum circuit model (QCM), (see *e.g.*, [60]), although the practical realization of it is yet to be found. Farhi and his collaborators [33] had proposed the adiabatic quantum computing (AQC) as an alternative, constructive model for implementing a quantum computer. They also propose an AQC algorithm for solving the 3-SAT problem which is one of the first identified NP-complete problems. But its running time is questioned by other theoretical physicists, for a phenomenon similar to Anderson localization [5] is believed to overshadow the usefulness of the proposed AQC algorithm. It was also realized that, from a computational complexity point of view, AQC is equivalent to all other models for universal quantum computation [1]. AQC as a model for universal quantum computation is also believed to be more robust than QCM because of the fact that quantum evolution is protected by a uniform spectral gap between the ground state energy and the rest energy levels, *e.g.*, see Adiabatic theorem 3.3.1 below.

Besides the NP-complete problems, the unstructured search problem is also of great interest, since it is perceived as a model of searching for an entry in a large database. The unstructured search problem can be formulated as the following: Given $F : \{0,1\}^n \to \{0,1\}$ and knowledge that there exists a unique element x such that $F(x) = 1$, find x. It is clear that classically, one needs to check $F(x)$ for all $N = 2^n$ values of x to find the solution, so the time complexity of doing so is $O(N)$. Grover's algorithm [38], originally derived in the framework of QCM, is one of the milestones in quantum computing. The ingenuity of the Grover's algorithm is that it uses a sequence of rotations that takes the initial state, which is a uniform superposition of all basis state, to the solution state. Originally the initial state is almost orthogonal to the solution state, *i.e.*, an angle of almost $\pi/2$. Now, each rotation in Grover's algorithm brings the initial state a radius of $1/\sqrt{N}$ closer to the solution state. As a result, the algorithm uses only $O(\sqrt{N})$ steps to achieve the result, in the framework of QCM. This bound is indeed proven to be optimal for query type quantum algorithms, see [11]. In the case where there are m (not necessarily 1) values of x for which $F(x) = 1$, a modified version of Grover's

algorithm works in QCM if the number m is known [14]. The technique for finding m is called quantum counting and was developed for QCM in [15].

The original motivation of introducing AQC was to derive the physically attainable algorithm for solving optimization problems such as satisfiability of Boolean formulas by encoding a cost function into the final Hamiltonian H_F. That is, one starts from an initial Hamiltonian and arrives at H_F by following a certain path, *i.e.*, $H(s) = (1 - f(s))H_I + f(s)H_F$ where f is an interpolating function. One of the (very few) models for which AQC had been shown to produce a speedup is Grover's search problem, addressed first in [34]. The further works in this direction (*e.g.* [69, 63]) considered the original problem of Grover (that is the case $m = 1$). The natural question that arises in this context is whether the Grover type running time, $O(\sqrt{N})$, is still optimal for a more general class of problem Hamiltonian, characterized by $N \gg m > 1$. That means that one wants to derive the analytic lower bound on the runtime of the algorithm, as well as to construct the suitable realization of the algorithm for which the running time (being the upper bound on the optimal time) is comparable with this lower bound. A partial result in this direction, namely the lower bound for some class of such models, was established in [42] (a detailed discussion will follow in section 3.1).

In this dissertation, a number of rigorous results are presented, mainly drawn from [17], concerning Hamiltonian-based quantum search problems that satisfy Assumption 2. The results include in particular upper and lower bounds on the amount of time needed to perform a general Hamiltonian-based quantum search, a lower bound on the evolution time needed to perform a search that is valid in the presence of control error and a generic upper bound on the minimum eigenvalue gap for evolutions.

The lower bound on the evolution time is, to our knowledge, the tightest for AQC type problems. It matches exactly the results established in the framework of the quantum circuit algorithm, when applied to Grover's search problem.

A specific Hamiltonian-based algorithm with the runtime $\tau = O(\sqrt{N/m})$ is presented, which nearly recovers the lower bound, and is thus close to being optimal in the case of Grover's search, where the final Hamiltonian is a rank m projection. The construction is augmented with a Hamiltonian-based quantum counting subroutine, which allows us to compute one of the more sensitive parameters, which is equivalent to the knowledge of the number of marked items, to the algorithm. Since the algorithm is robust in a sense that we can allow the running time to vary in a large time interval, it is less sensitive to the ground state energy E_F, which is the other parameter that shows up in the proposed algorithm. As a result, only an approximate knowledge of E_F is needed to ensure that the algorithm works, and estimation on this parameter is not considered here.

In a realistic setting, one needs to take into account the control constraint. The result presented here assumes the interpolating function f has a velocity $\dot{f}$ that is greater than a fixed control parameter κ during the evolution, excluding the vicinities of the endpoints $s = 0, 1$ where it is allowed to be small. We show that the necessary control accuracy requirement should be at least $O(\ln N/\sqrt{N})$ for the algorithm to succeed. In particular,

this result implies that the starting slow / finishing slow strategy, *e.g.*, proposed in [72], by itself is not sufficient to make AQC better than the classical computer. One really needs to investigate closely the large bulk of time that the Adiabatic evolution spent in the middle of the path to be able to get any quantum speedup.

Finally, because of the general interest in the spectral gap of the interpolating Hamiltonian for AQC, an upper bound on the size of the first spectral gap for this family of matrices is presented, even though none of the main results presented used the knowledge of the gap structure of the underlying interpolating Hamiltonian $H(s)$. The result is that for the final Hamiltonian of the Grover's type, *i.e.*, when H_F is a rank m projection, the smallest value of the gap cannot exceed $O(\sqrt{m/N})$. The technique presented can be also used to find a lower bound on the gap.

For a general form of H_F, *e.g.*, when it is not assumed to be of finite rank, no general lower bounds on the runtime can be obtained, as the examples constructed in [22] show. It is still a relatively open problem to establish "typical" lower and upper bounds for the random instances of NP-complete problems, as discussed in [5].

1.4 Some series expansion formulas

It often happens that, common mathematical techniques are used to tackle problems arising from seemingly completely different fields. In this dissertation, the interesting technique is series expansion and it deserves a few words in the beginning.

The most common and straightforward expansion technique is arguably Taylor's expansion, which has the form

$$f(x+h) = f(x) + hf'(x) + \frac{h^2 f''(x)}{2} + \cdots + \frac{h^n f^{(n)}(x)}{n!} + o(h^n).$$

The requirement for the expansion to hold is that $f(x)$ is n-times differentiable at a vicinity of x, namely ball $B(x;\epsilon)$, that includes $x+h$.

Then there is the Fourier expansion of a continuous and periodic function

$$f(x) = c_0 + c_1 e^{2\pi i x} + c_2 e^{4\pi i x} + \cdots + c_n e^{2n\pi i x} + \cdots$$

where $c_n = \int_0^1 f(x) e^{2n\pi i x} dx$ given the period of function f is 2.

For any bounded operator H_0 and V, let $H = H_0 + \lambda V$ and suppose $R = H^{-1}$ and $R_0 = H_0^{-1}$ exist, the first resolvent identity is

$$R = R_0 + R_0 \lambda V R = R_0 + R \lambda V R_0.$$

The series can be expanded to arbitrary order, so

$$R = \sum_{i=0}^{N} (-R_0 \lambda V_\omega)^i R_0 + (-R_0 \lambda V_\omega)^{N+1} R.$$

The second resolvent identity is

$$R = \sum_{i=0}^{\infty} (-R_0 \lambda V_\omega)^i R_0.$$

This is true when $\|\lambda V\| < 1$, and the convergence is in the strong norm sense.

If H_0 is the discrete Laplacian operator and V is a multiplication operator with diagonal element randomly distributed, one can take expectation $\mathbb{E}[\langle xHy \rangle]$. Later we'll see that a modified decomposition of H together with a renormalization and Feynman diagrammatic technique will allow us to get tight control on this quantity, and that is a key element to the proof of weak localization discussed in this dissertation.

Given a Schrödinger equation, one can write out the Duhamel expansion. Consider the unitary evolution given by

$$i\frac{d}{dt}U(t,0) = H(t)U(t,0); \quad U(0,0) = I, t \in [0,\tau] \tag{1.9}$$

Now let's rescale the evolution by $s = t/\tau$, and we get

$$i\frac{d}{ds}U_\tau(s,0) = \tau H_\tau(s)U_\tau(s,0); \quad s \in [0,1] \tag{1.10}$$

The Duhamel expansion stopped at order 2 is the following

$$\begin{aligned} U_\epsilon(s,0) &= I - i\tau \int_0^s H_\tau(r)U_\tau(r,0)dr & (1.11)\\ &= I - i\tau \int_0^s H_\tau(r)dr + (-i\tau)^2 \int_0^s H_\tau(r) \int_0^r H_\tau(l)U_\tau(l,0)dl & (1.12) \end{aligned}$$

One application of this expansion is used in the investigation of the running time of a Hamiltonian evolution in part 2.

There is another representation for the same quantum evolution, namely, the Heisenberg equation,

$$i\frac{d}{ds}P_\tau(s) = \tau[H(s), P_\tau(s)] \tag{1.13}$$

where $P_\tau(s)$ is the projection onto the wave function $\psi_\tau(s)$. Let's further assume the ground energy $E(s)$ is uniformly isolated from the rest, and that $P_\tau(0)$ is the projection onto the ground state of $H(0)$. It turns out that although it is not easy to decompose $\psi_\tau(s)$ into an asymptotic series in powers of τ^{-1}, a power expansion for $P_\tau(s)$ exists and is originally proposed by Nenciu [59]

$$P_\tau(s) = B_0(s) + \frac{1}{\tau}B_1(s) + \frac{1}{\tau^2}B_2(s) + \cdots \tag{1.14}$$

where $B_0(s) = P(s)$, the projection onto the ground state of $H(s)$, and $B_j(s)'s$ are recursively given by

$$B_j(s) = \frac{1}{2\pi}\int_\Lambda R_z(s)[P(s), \frac{d}{ds}B_{j-1}(s)]R_z(s)dz + S_j(s) - 2P(s)S_j(s)P(s) \tag{1.15}$$

where $R_z = (H(s) - z)^{-1}$, $S_j(s) = \sum_{m=1}^{j-1} B_m(s)B_{j-m}(s)$, and the contour Λ only encircles the ground energy. A. Elgart and G. Hagedorn [27] utilized Nenciu's expansion to derive an lower bound on the adiabatic running time when the adiabatic error is of size $o(1)$ given the Hamiltonian belongs to the Gevrey class G^α.

Chapter 2

Weak localization for the alloy-type Anderson model on a cubic lattice

2.1 Assumptions and main results

The Hamiltonian H_ω^λ on the vector $\psi \in l^2(\mathbb{Z}^3)$ under consideration is described in equation below:

$$(H_\omega^\lambda \psi)(x) \;:=\; -\frac{1}{2}\,(\Delta\psi)(x) + \lambda V_\omega(x)\psi(x)\,. \tag{2.1}$$

Here Δ denotes the discrete Laplace operator,

$$(\Delta\psi)(x) \;=\; \sum_{e\in\mathbb{Z}^3,\ |e|=1} \psi(x+e) \;-\; 6\psi(x)\,, \tag{2.2}$$

and V_ω stands for a random multiplication operator of the form

$$V_\omega(x) \;=\; \sum_{i\in\mathbb{Z}^3} \omega_i\, u(x-i)\,. \tag{2.3}$$

The parameter λ conveniently describes the strength of disorder.

2.1.1 Assumptions

Randomness

($\mathcal{A}$) The values of the random potential $\{\omega_i\}$ are i.i.d. variables, with a bounded probability density ρ that is even, compactly supported on an interval J. We will further assume (without loss of generality) that J is centered around the origin and that the second moment satisfies $\mathbb{E}\,\omega_i^2 = 1$. The function ρ is Liftshitz continuous:

$$|\rho(x) - \rho(y)| \;\leq\; K|x-y|\,\max(\mathbf{1}_J(x), \mathbf{1}_J(y)\,), \tag{2.4}$$

where $\mathbf{1}_I$ stands for a characteristic function of the set I.

Single site potential

We will impose rather mild conditions on the *single site potential* function u. Namely, we will assume that $u(x)$ decays exponentially fast:

$$|u(x)| \;\leq\; Ce^{-A|x|}\,. \tag{2.5}$$

Notation and quantities of interest

In what follows we will denote by $A(x,y)$ the kernel of the linear operator A acting on $l^2(\mathbb{Z}^3)$ (that is $A(x,y) = (\delta_y, A\delta_x) = \langle y|A|x\rangle$, where δ_x is an indicator function of the site $x \in \mathbb{Z}^3$, and $(\cdot,\cdot)$ denotes the inner product of $l^2(\mathbb{Z}^3)$). We will use the concise notation $\int$ in place of $\int_{(\mathbb{T}^3)^k}$ whenever it is clear from the context.

The dissertation investigates the properties of H^λ_ω for a typical configuration ω in a weak disorder regime, namely at the energy range $E < E_0$, where

$$E_0 \;=\; -2\lambda^2\|\hat{u}\|^2_\infty - 2\lambda^4\|\hat{u}\|^4_\infty\,, \tag{2.6}$$

for $\lambda > 0$ being sufficiently small.

The quantity of the most interest is the typical asymptotic behavior of the Green function (also known as the two point correlation function, the propagator)

$$R_{E+i\epsilon}(x,y) \;=\; (H^\lambda_\omega - E - i\epsilon)^{-1}(x,y) \tag{2.7}$$

in the limit $\epsilon \searrow 0$.

Diagramatic expansion and self energy

The technical assertions are proven using a Feynman diagrammatic expansion for $R_{E+i\epsilon}$ around the unperturbed resolvent, *i.e.*, the one with $\lambda = 0$. The rate of convergence for this expansion in the limit $\epsilon \to 0$ depends strongly on the value of E, and sets our limitations for the length of the interval I where we can prove localization. One can eliminate certain terms in this expansion (the so called tadpole contributions) that are especially problematic from the convergence point of view, by modifying the unperturbed Hamiltonian. The corresponding addend σ is called the *self energy* of the model.

Define the self energy by the solution of the self-consistent equation

$$\sigma(p, E+i\epsilon) \;=\; \lambda^2 \int_{\mathbb{T}^3} d^3q\, \frac{|\hat{u}(p-q)|^2}{e(q) - E - i\epsilon - \sigma(q, E+i\epsilon)}\,. \tag{2.8}$$

The relevant properties of the solution of (2.8) are collected in Appendix 2.5.2. In particular, it has a single valued solution $\sigma(p, E + i\epsilon)$ for all ϵ, all $p \in \mathbb{T}^3$ and all values of E that meet the condition (2.6). The function σ satisfies

$$\|\sigma\|_\infty \;\leq\; 2\lambda^2 \|\hat{u}\|_\infty^2.$$

2.1.2 Main result

The hallmark of localization is a rapid decay of the Green function at energies in the spectrum of H_ω, for the typical configuration ω. This behavior can be linked to the non-spreading of wave packets supported in the corresponding energy regimes and various other manifestations of localization. Our main result, Theorem 2.1.1 below, establishes this behavior of the Green function at the band edges of the spectrum, by comparing it with the asymptotics of the free Green function.

Theorem 2.1.1 (Anderson Localization for Lifshitz tails regime)**.** *For H_ω^λ as above that satisfies Assumption ($\mathcal{A}$), for any $\nu > 0$ there exists $\lambda_0(\nu)$ such that for all $\lambda < \lambda_0(\nu)$ the spectrum of H_ω within the set $E \leq E_0 - \lambda^{4-\nu}$ is almost-surely of the pure-point type, and the corresponding eigenfunctions are exponentially localized.*

2.1.3 Discussion

It should be noted that the method works most effectively when the average $\bar{u}$ of the single site potential is not equal to zero. In this case $\inf \sigma(H_\omega^\lambda) \leq C\lambda$ almost surely, with $C < 0$ (see Section 5.1 of [50]). Hence for λ sufficiently small, Theorem 2.1.1 establishes the localization at the bottom of the spectrum of H_ω^λ. We are only aware of one result on the Anderson localization in the regime discussed here for a non sign definite single site potential: F. Klopp proved the weak disorder localization for $E < -\lambda^{7/6}$ in three dimensions [51]. Since for $\bar{u} = 0$ case $-\inf \sigma(H_\omega^\lambda) = O(\lambda^2)$, his result does not provide an answer on whether the bottom of the spectrum is localized or not.

When the average of the single site potential vanishes, we expect the method to yield the non trivial result when the minimizing configurations of the random potential look flat. That is essentially a reason why we can cover say the dipole potential below, the observation we owe to Günter Stolz. In this case, the expansion around the free Green function is a sensible procedure to do.

In this dissertation, the cubic lattice is considered, that is $d = 3$ case. Similar (in fact better) results can be established for a higher dimensional case, but not for $d < 3$. Mathematically, it is related to the nature of the point singularity of the propagator $e(p)$ at zero energy - it is integrable for $d \geq 3$. This fact allows us to control the underlying Feynman series.

Finally, the discussion is ended with an example pertaining to the case $\hat{u}(0) = 0$ where the technique presented here allows to get a meaningful result by improving the bound on the threshold energy E_0:

Consider the single site potential u_d of the dipole type, *i.e.*,

$$u_d(x) \;=\; \begin{cases} 1 & x = 0 \\ -1 & x = e_1 \\ 0 & \text{otherwise} \end{cases} . \tag{2.9}$$

Proposition 2.1.2. *For the single site potential u_d and any random potential satisfying assumption $(\mathcal{A})$ in Subsection 2.1.1, we have*

$$\inf \sigma(H_\omega^\lambda) \;<\; -2\lambda^2 + O(\lambda^3)$$

almost surely. The statement of Theorem 2.1.1 holds true for all energies E that satisfy

$$E < E_d \;:=\; -(1+\lambda)\lambda^2 .$$

Remark 3. The proof of Proposition 2.1.2 is in Appendix 2.5.3. In fact, the first statement of Proposition 2.1.2 holds true for any probability measure $\mathbb{P}_0$ of random potential such that $\{1, -1\} \subset \mathrm{supp}\mathbb{P}_0$. The requirement $\mathbb{E}\,\omega_i^2 = 1$ we impose in assumption $(\mathcal{A})$ ensures this condition. For probability measure satisfying $\{-C, C\} \subset \mathrm{supp}\mathbb{P}_0$, one can use a scaling argument, *i.e.*, $\omega \to \frac{1}{C}\omega$ and $\lambda \to C\lambda$, to see

$$\inf \sigma(H_\omega^\lambda) \;<\; -2C^2\lambda^2 + O(\lambda^3).$$

2.2 Renormalization technique

As mentioned earlier, the quantity of interest is the Green function and it's typical asymptotic behavior. More specifically, one wants to compute $\mathbb{E}[R_{E+i\epsilon}(x,y)]$. Remember $H_\omega^\lambda = -\frac{1}{2}\Delta + \lambda V_\omega$. A first attempt is to expand H_ω^λ as

$$R = \sum_{i=0}^{N} (-R_0 \lambda V_\omega)^i R_0 \;+\; (-R_0\lambda V_\omega)^{N+1} R . \tag{2.10}$$

where $R_0 = (-\frac{1}{2}\Delta - E - i\epsilon)^{-1}$ and the subscript in $R_{E+i\epsilon} = (H_\omega^\lambda - E - i\epsilon)^{-1}$ is omitted. So

$$\mathbb{E}[(-R_0\lambda V_\omega)^n R_0(x_0, x_{n+1})] \;=\; \mathbb{E}\Big[\sum_{x_k \in \mathbb{Z}^3; k=1,\dots,n} \prod_{j=1}^{n} (-\lambda V_\omega(x_j)) \prod_{i=0}^{n} R_0(x_i, x_{i+1}) \Big] \tag{2.11}$$

$$\;=\; (-\lambda)^n \sum_{x_k \in \mathbb{Z}^3; k=1,\dots,n} \mathbb{E}\Big[\prod_{j=1}^{n} V_\omega(x_j) \Big] \prod_{i=0}^{n} R_0(x_i, x_{i+1}) \tag{2.12}$$

In the following we investigate

$$\mathbb{E}\Big[\prod_{j=1}^{n} V_\omega(x_j)\Big].$$

First, assume $u(x-i)=\delta_x(i)$, so $V_\omega(x_j)=w_{x_j}$. For an integer N, let Υ_N be a set $\{1,\dots,N,N+2,\dots,2N+1\}$. Let $\Pi=\Pi_N$ be a set of partitions of Υ_N into disjoint subsets S_j of cardinality $|S_j|\in 2\mathbb{N}$. Two partitions $\pi=\{S_j\}_{j=1}^m$, $\pi'=\{S'_j\}_{j=1}^m$ are equivalent, $\pi=\pi'$, if they coincide up to permutation. For $S\subset\Upsilon_N$, let

$$\delta(x_S)=\sum_{y\in\mathbb{Z}^3}\prod_{j\in S}\delta(x_j-y)\,, \tag{2.13}$$

where x_S denotes the collection of $\{x_i\,,\ i\in S\}$. One has an identity (see *e.g.* [18] Section 3.1 for details)

$$\mathbb{E}\left[\prod_{j\in\Upsilon_N}\omega_{x_j}\right]=\sum_{m=1}^{N}\sum_{\pi=\{S_j\}_{j=1}^m}\prod_{j=1}^{m}c_{|S_j|}\delta(x_{S_j})\,, \tag{2.14}$$

where $c_{2l}\le(cl)^{2l+1}$ and $c_2=\mathbb{E}\,\omega_x^2=1$, provided assumption $(\mathcal{A})$ holds. The set S_j in the partitions $\pi\in\Pi$ can be of the special type: If

$$S_j=\{i,i+1\} \tag{2.15}$$

we will refer to it as a *tadpole*, or a *gate* set. The contributions from the terms that contains gates are particular troublesome because they give rise to

$$\int\frac{dp_i}{(e(p_i)+E)^2}\sim\int\frac{r^2\cos\theta}{(e(p_i)+E)^2}drd\theta d\alpha\sim C\frac{1}{\sqrt{E}}$$

as apposed to the more favorable term

$$\Big(\int\frac{dp_i}{e(p_i)+E}\Big)^2\sim C$$

in the momentum representation. The worst possible tadpole term comes from the partition $\pi=\{\{1,2\},\dots,\{N-1,N\},\{N+2,N+3\},\dots,\{2N,2N+1\}\}$ and it leads to

$$\int\frac{dp_i}{(e(p_i)+E)^{2N}}\sim C\frac{1}{E^{2N-3/2}}$$

The aim of the renormalization technique is to get rid of those tadpole terms. To this end, let's do the following decomposition:

$$H_\omega^\lambda=H_r+\tilde V\,,\quad H_r:=-\frac{1}{2}\Delta-\sigma(E+i\epsilon)\,,\quad \tilde V:=\lambda V_\omega+\sigma(E+i\epsilon)\,.$$

Then the corresponding resolvent expansion for R becomes

$$R = \sum_{i=0}^{N} (-R_r \tilde{V})^i R_r \;+\; (-R_r \tilde{V})^{N+1} R\,, \tag{2.16}$$

where $R_r = (H_r - E - i\epsilon)^{-1}$.

To handle the renormalization of tadpole contributions properly, we decide at which value of n to halt the expansion in (2.16) individually for each contribution according to the following rule (to which we will refer as a stopping rule): If we open the brackets in (2.16), we obtain terms of the form

$$R_r \theta R_r \theta \ldots R_r \theta R_r$$

where θ is either $-\lambda V_\omega$ or $-\sigma(E + i\epsilon)$ (whenever θ takes the later value we will refer to it as a *bullet*). Since $\sigma(E + i\epsilon) = O(\lambda^2)$, for all permissible values of E, see Appendix 2.5.2, one can unambiguously define the *order* l (in powers of λ) of the particular contribution

$$R_r \theta R_r \theta \ldots R_r \theta R_\sharp\,,$$

(with $R_\sharp$ being either R_r or R) according to the following rule: Each factor of σ counts as 2, while appearance of the random potential counts as 1, and we add up all the exponents to get the order of the term. For instance, the order of the expression

$$R_r \sigma R_r \lambda V_\omega R_r \sigma R$$

is 5. To illustrate this procedure we write down the expansion obtained in a case of $N = 2$:

$$\begin{aligned} R \;&=\; R_r \;-\; R_r \sigma R \;-\; \{\lambda R_r V_\omega R\} \\ &=\; R_r \;-\; R_r \sigma R \;-\; \lambda R_r V_\omega R_r + \; \lambda R_r V_\omega R_r \sigma R \;+\; \lambda^2 R_r V_\omega R_r V_\omega R\,, \end{aligned}$$

where the term in the curled brackets is the one we expanded according to the stopping rule. Note that the penultimate term is of order 3. It is not difficult to see (see Lemma 3.1 in [26] for the proof) that for a general N we get

Lemma 2.2.1. *For any integer N we have a decomposition*

$$R \;=\; \sum_{l=0}^{N-1} A'_l R_r + A'_N R + B_N R \;=\; \sum_{l=0}^{N-1} A_l \;+\; \tilde{A}_N R\,, \tag{2.17}$$

where $A'_0 = I$, A'_l is a summation over all possible terms of the type

$$R_r \theta R_r \theta \ldots R_r \theta \tag{2.18}$$

which are of the order $l > 0$, while

$$B_N \;=\; -\,A_{N-1}\sigma\,. \tag{2.19}$$

The quantities A_l and $\tilde{A}_N$ are defined as

$$A_l \;=\; A'_l R_r\,, \quad \tilde{A}_N \;=\; A'_N + B_N\,.$$

Now let π_k^c denote a collection of disjoint sets $\{S_j\}$ such that any $S_j \in \pi_k^c$ is a tadpole, and the cardinality of π_k^c is k. Then any partition π can be decomposed as $\pi = \pi_k^c \cup \{S\}$ for some $0 \leq k \leq N$, where S satisfies $(\cup_{s_j \in \pi_k^c} S_j) \cup S = \Pi_N$. Note that we didn't require S to be a tadpole free set. We will denote by π_0 a partition of Υ_N such that no $S_j \in \pi_0$ is a tadpole. Then we have the following observation:

$$\sum_{k=0}^{N}(-1)^k \sum_{\substack{\pi\in\Pi:\\ \pi=\pi_k^c\cup\{S\}}} \mathbb{E}\left[\prod_{i\in S}\omega_{x_i}\right] \prod_{S_l\in\pi_k^c}\delta(x_{S_l}) \;=\; \sum_{\substack{\pi\in\Pi:\\ \pi=\pi_0}} \prod_{S_j\in\pi} c_{|S_j|}\delta(x_{S_j})\,. \tag{2.20}$$

Note that the summation on the right hand side runs over the tadpole-free partitions. To verify (2.20) one just need to make a straightforward check that all tadpole contributions on the left hand side cancel out exactly.

When the single site potential $u(x-i) = \delta_x(i)$, we have:

Lemma 2.2.2.

$$\mathbb{E}A_l^2(x,y) \;=\; \lambda^{2l} \sum_{\substack{\pi\in\Pi_l:\\ \pi=\pi_0}} \sum_{\substack{x_j\in\mathbb{Z}^3:\\ j\in\Upsilon_l}} \prod_{S_j\in\pi} c_{|S_j|}\delta(x_{S_j}) R_r(x,x_1)R_r(x,x_{l+2}) \prod_{i\in\Upsilon_l} R_r(x_i,x_{i+1}) \tag{2.21}$$

where we are using convention $x_0 = x$; $x_{2l+2} = y$.

The renormalization also carries over to the case with the general single site potential u considered in this dissertation. The counterpart of Lemma 2.2.2 in this case is the following generalization of Lemma 3.2 of [26]. In what follows, we will use the short hand notation $E(p)$ in place of $e(p) - E - i\epsilon - \sigma(p, E+i\epsilon)$, and $E^*(p)$ for the hermitian conjugate of the multiplication operator $E(p)$. The renormalized propagator R_r in this case will be given by its kernel

$$R_r(z,w) \;=\; \int_{\mathbb{T}^3} e^{i2\pi(z-w)p} \frac{d^3p}{E(p)}\,. \tag{2.22}$$

The following assertion holds:

Lemma 2.2.3. *For A_l defined in Lemma 2.2.1, the function $\mathbb{E}\,|A_l(x,y)|^2$ is a function of the variable $x-y$. Let*

$$\mathcal{A}_{l,E}(x-y) \;:=\; \mathbb{E}\,|A_l(x,y)|^2\,, \tag{2.23}$$

then we have

$$\begin{aligned}\mathcal{A}_{l,E}(x-y) \;=\; \lambda^{2l} \int_{(\mathbb{T}^3)^{2l+2}} e^{i\alpha}\, \frac{dp_{l+1}}{E(p_{l+1})}\,\frac{dp_{2l+2}}{E^*(p_{2l+2})} \prod_{j=1}^{l}\frac{dp_j}{E(p_j)} \prod_{j=l+2}^{2l+1}\frac{dp_j}{E^*(p_j)} \\ \times \prod_{i\in\Upsilon_l}\hat{u}(p_j-p_{j+1}) \sum_{\substack{\pi\in\Pi_l:\\ \pi=\pi_0}} \prod_{S_k\in\pi} c_{|S_k|}\,\delta\left(\sum_{i\in S_k} p_i - p_{i+1}\right)\,,\end{aligned} \tag{2.24}$$

where

$$\alpha \;:=\; -i2\pi(p_1+p_{l+2})\cdot(x-y)\,.$$

Proof.

Let V_ω^δ be a random potential of the form

$$V_\omega^\delta(x) \;=\; \sum_{i\in k\mathbb{Z}^3}\omega_i e^{-\delta|i|}\,u(x-i)\,.$$

Then $V_\omega^\delta \longrightarrow V_\omega$ in the strong operator topology as δ converges to 0. Similarly, we can define quantities $H_\omega^{\lambda,\delta}$, R^δ, R_r^δ, and A_l^δ by replacing V_ω with V_ω^δ. One can readily check that

$$R^\delta(x,y)\to R(x,y)\,;\quad R_r^\delta(x,y)\to R_r(x,y)\,,\quad A_l^\delta(x,y)\to A_l(x,y)$$

in the limit $\delta\to 0$. The advantage of working with the regularized random potential is due to the fact that it is summable and therefore admits Fourier transform. Namely, we have

$$\hat V_\omega^\delta(p) \;=\; \hat u(p)\,\hat\omega_\delta(p)\,,$$

where

$$\hat\omega_\delta(p) \;:=\; \sum_{n\in\mathbb{Z}^3} e^{-i2\pi p\cdot n}\,\omega_n\,e^{-\delta|n|}\,.$$

Since by (2.8) we have

$$\lambda^2\int_{\mathbb{T}^3}|\hat u(p-q)|^2\,R_r(q)dq \;=\; \sigma(p,E+i\epsilon)\,,$$

we can express $\mathbb{E}|A_l^\delta(x,y)|^2$ as

$$\begin{aligned}\mathbb{E}|A_l^\delta(x,y)|^2 \;=\;&\\ \lambda^{2l}\int_{(\mathbb{T}^3)^{2l+2}} e^{i\beta}\,&\frac{dp_{l+1}}{E(p_{l+1})}\,\frac{dp_{2l+2}}{E^*(p_{2l+2})}\,\prod_{j=1}^{l}\frac{dp_j}{E(p_j)}\,\prod_{j=l+2}^{2l+1}\frac{dp_j}{E^*(p_j)}\,\prod_{i\in\Upsilon_l}\hat u(p_j-p_{j+1})\\ &\times\sum_{k=0}^{N}(-1)^k\sum_{\substack{\pi\in\Pi_l:\\ \pi=\pi_k^c\cup\{S\}}}\mathbb{E}\left[\prod_{i\in S}\hat\omega_\delta(p_i-p_{i+1})\right]\prod_{S_l\in\pi_k^c}\delta\left(\sum_{i\in S_l}p_i-p_{i+1}\right)\,, \qquad (2.25)\end{aligned}$$

where $\beta:=2\pi\{-(p_1+p_{l+2})\cdot x+(p_{l+1}+p_{2l+2})\cdot y\}$. It follows from (2.20) that

$$\begin{aligned}\sum_{k=0}^{N}(-1)^k\sum_{\substack{\pi\in\Pi_l:\\ \pi=\pi_k\cup\pi_k^c}}\prod_{S_l\in\pi_k^c}\delta\left(\sum_{i\in S_l}p_i-p_{i+1}\right)\,\mathbb{E}\left[\prod_{i\in S_j\in\pi_k}\hat\omega_\delta(p_i-p_{i+1})\right]&\\ \xrightarrow{d}\sum_{\substack{\pi\in\Pi:\\ \pi=\pi_0}}\prod_{S_j\in\pi}c_{|S_j|}\delta\left(\sum_{i\in S_j}p_i-p_{i+1}\right)\,,&\end{aligned}$$

where $\xrightarrow{d}$ stands for the convergence (with respect to δ) in the distributional sense. Therefore, taking the expected value on the both sides of (2.25) as well as $\delta \to 0$ limit (where we use the smoothness of the integrand), we arrive to the expression that coincides with (2.24), up to the prefactor $e^{i\beta}$ instead of $e^{i\alpha}$ in the integrand. But the product of the delta functions forces $\delta(p_1 - p_{l+1} + p_{l+2} - p_{2l+2})$ (see Subsection 2.3 below), so we can replace β with α, hence the result.

□

2.3 Estimation on the decomposition of $R(x, y)$

In this subsection we establish the estimates on the decomposition of $R(x, y)$ given in Equ. 2.17. We introduce some additional notation first. δ will be a very small parameter that's roughly $\sqrt{E^*}$, and we would impose on E the condition

$$E \leq -4\pi^2\delta^2 - 2\lambda^2(\|\hat{u}\|_\infty + 4\pi C A^{-4}\delta)^2 - E^*. \tag{2.26}$$

Details follow later in this subsection and next subsection.

We will denote by $G_E(x, y)$ the free Green function, *i.e.*,

$$G_E(x, y) \;:=\; \langle x| \, (-\Delta/2 - E)^{-1} \, |y\rangle \, . \tag{2.27}$$

We characterize its relevant properties in Appendix 2.5.1. It will be used in some of the proofs as comparison with the full Green function $R_{E+i\epsilon}(x, y)$, defined in (2.7). Whenever it is clear from the context, we will suppress the energy dependence of $R_{E+i\epsilon}$, and just use R (respectively $R(x, y)$) for the full resolvent (the full Green function).

Lemma 2.3.1 (Decomposition of $R(x, y)$)**.** *For any integer N and energies $E < E_0$ with E_0 satisfying* (2.6) *we have the decomposition*

$$R(x, y) \;=\; \sum_{n=0}^{N-1} A_n(x, y) \;+\; \sum_{z \in Z^3} \tilde{A}_N(x, z) R(z, y) \, , \tag{2.28}$$

with $A_0(x, y) = R_r(x, y)$ (the latter kernel is defined in (2.22) *above), and where the (real valued) kernels A_n, $\tilde{A}_N$ satisfy bounds*

$$\mathbb{E}\,|A_n(x, y)|^2 \;\leq\; (4n)!\, E^* \left(C(E^*) \, \frac{\lambda^2}{\sqrt{E^*}} \right)^n \, e^{-\delta\,|x-y|} \, , \quad n \geq 1 \, ; \tag{2.29}$$

$$\mathbb{E}\,|\tilde{A}_N(x, y)| \;\leq\; \sqrt{(4N)!} \left(C(E^*) \, \frac{\lambda^2}{\sqrt{E^*}} \right)^{N/2} \, e^{-\delta|x-y|/2} \, , \quad N > 1 \, ; \tag{2.30}$$

where

$$C(E^*) \;=\; K \left(\|\hat{u}\|_\infty \,+\, 4\pi C A^{-4}\delta \right)^2 \, \ln^9(E^*)$$

for some generic constant K, and C, A are parameters introduced in (2.5).

The zero order contribution A_0 satisfies

$$|A_0(x,y)| \;\leq\; e^{-\frac{\delta}{\sqrt{3}}|x-y|} \tag{2.31}$$

for all $x, y \in \mathbb{Z}^3$.

One then looks for the optimal value N to stop the corresponding expansion - note that the increasing factor of $(4N)!$ in $A_N(x,y)$ competes with the decreasing factor $(\lambda^4/E^*)^{N/2}$.

The choice $E^* = \lambda^{4-\nu}/2$ has the effect that

$$C(E^*)\,\frac{\lambda^2}{\sqrt{E^*}} \;\leq\; \lambda^{B\nu}\,, \quad 0 < B < 1\,, \tag{2.32}$$

which suffices to control (2.29) – (2.30)). We note that in the range of energies $E < E_0 - \lambda^{4-\nu}$, the condition (2.26) and the above choice for E^* implies $\delta^2 > \lambda^{4-\nu}/(4\pi)^2$. It turns out that the appropriate choice for N should satisfy

$$(4N)!\,\left(\frac{C(E^*)\lambda^2}{\sqrt{E^*}}\right)^N \approx e^{-N}$$

(see the next section for details). In terms of the λ - dependence, it corresponds to $N \sim \lambda^{-b\nu}$ for $b < B$.

At this point we have to introduce some additional notation:

Definition 1. We consider products of delta functions with arguments that are linear combinations of the momenta $\{p_1, p_2, \ldots, p_{2n+2}\}$. Two products of such delta functions are called *equivalent* if they determine the same affine subspace of $\mathbb{T}^{2n+2} = \{p_1, p_2, \ldots, p_{2n+2}\}$.

One can obtain new delta functions from the given ones, by taking linear combinations of their arguments. In particular, we can obtain identifications of momenta.

Definition 2. The product $\delta(\sum_j a_j p_j)$ of delta functions Δ_π *forces* a new delta function, if $\sum_j a_j p_j = 0$ is an identity in the affine subspace determined by Δ_π.

One can readily see that in the integrand of rhs of (2.24) one has a forced delta function $\delta(p_1 - p_{l+1} + p_{l+2} - p_{2l+2})$, the fact used in Lemma 2.2.3.

$A_{l,E^*}(x-y)$ is conveniently interpreted in terms of the so called Feynman graphs (the pseudograph, to be precise, since loops and multiple edges are allowed here). The graph, associated with particular partition π of $\Upsilon_{n,n}$ is constructed according to the following rules (see Figure 2.1 and 2.2): We first draw two line segments, each containing n vertices (elements of $\Upsilon_{n,n}$). The vertices are joined by directed edges (momentum lines) representing the corresponding

momenta: $p_1, \ldots, p_{n+1}$ and $p_{n+2}, \ldots, p_{2n+2}$. To each line p_j we assign a propagator $F(p_j)$, with some given function F, save momentum lines p_1 and p_{n+2}, which carry additional phases $e^{-i2\pi p_1 \cdot (x-y)}$ and $e^{-i2\pi p_{n+2} \cdot (x-y)}$, respectively. For $\pi = \{S_j\}_{j=1}^m$ we identify all vertices in each subset S_j as the same vertex (in Figure 2.1, the paired vertices are connected by dashed lines).

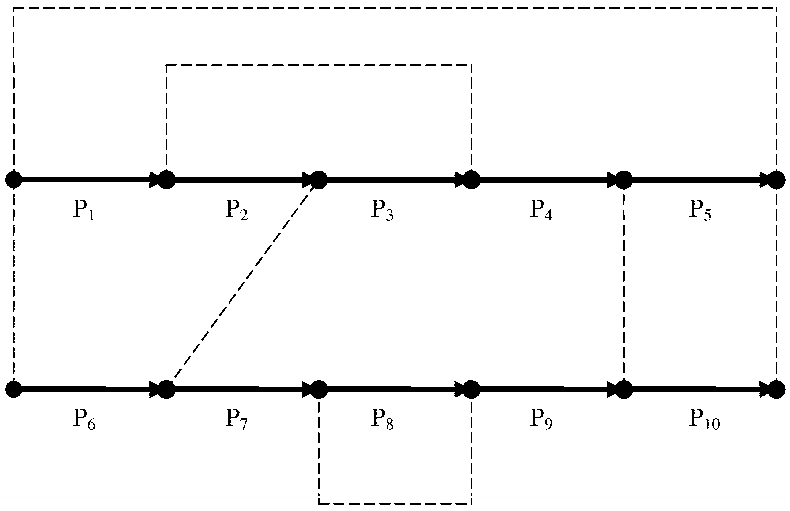

Figure 2.1: Construction of the Feynman graph, part I, $n = 4$. The corresponding delta functions are $\delta(p_1 - p_2 + p_3 - p_4)$, $\delta(p_4 - p_5 + p_9 - p_{10})$, $\delta(p_2 - p_3 + p_6 - p_7)$, and $\delta(p_7 - p_9)$. The last delta corresponds to the tadpole. Note that the sum of all momenta in the above delta functions gives a forced delta function $\delta(p_1 - p_5 + p_6 - p_{10})$, hence we can introduce the dashed lines connecting vertices $1, 6, 7$, and 12, identifying them as a single vertex.

Note that thanks to the existence of the forced delta function $\delta(p_1 - p_{l+1} + p_{l+2} - p_{2l+2})$, we can identify vertices $1, l, l+1, 2l$ as a single one, and therefore one can think about the closed graph (with special rules that apply for momentum lines p_1 and p_{l+2}, mentioned above). To summarize, the outcome of this construction is a directed closed graph, which is called the Feynman graph associated with the partition π. The momenta in the graph satisfy the Kirchhoff's first law, that is the total momenta entering into each internal vertex add up to zero (if arrow faces outward the vertex, we count its momentum with a minus sign). A tadpole corresponds to the so-called 0-*loop*, that is some (directed) line of the graph claims one vertex as its both endpoints. For a given Feynman graph G, one can choose a particularly useful expression for the product of delta functions Δ_π. Choose any spanning tree of G which does not contain momentum lines p_1, p_{l+2}. The edges belonging to the spanning tree will be called the *tree* edges (momentum lines), and all the rest are the *loop* edges (since an addendum of any loop's momentum line creates a loop). Let us enumerate the tree variables as $u_1, ..., u_k$, and loop variables as $w_1, ..., w_n$, with say $w_1 = p_1, w_2 = p_{l+2}$ (note that $k + n = 2l + 2$). The number k of the tree momenta coincides with the number of the delta functions in Δ_π.

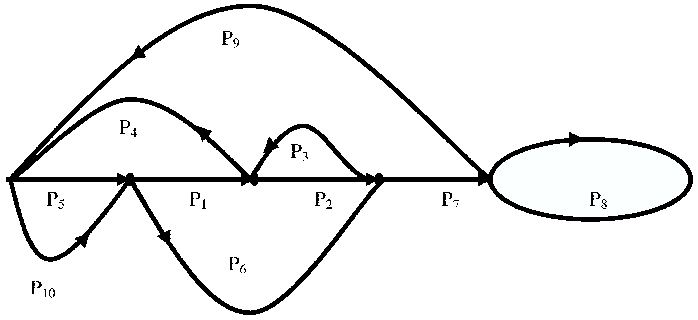

Figure 2.2: Construction of the Feynman graph, part II: Identification of the vertices. The tadpole corresponds here to 0-loop.

One can check (see *e.g.* [32]) that the product of delta functions Δ_π is equivalent to

$$\prod_{i=1}^{k} \delta(u_i - \sum_{j=1}^{l} a_{ij} w_j)\,, \tag{2.33}$$

with

$$a_{ij} := \begin{cases} \pm 1 & \text{loop that contains } u_i \text{ is created by adding } w_j \text{ to the spanning tree} \\ 0 & \text{otherwise} \end{cases}.$$

The choice of the sign depends on the mutual orientation of u_i and w_j.

Proof of Lemma 2.3.1.

We establish the exponential decay of $\mathcal{A}_{l,E}(x-y)$ in $|x-y|$ from the following analytic argument. To this end we generalize the arguments used in Section 4. of [26] to the *momentum–dependent* self energy σ (defined in Eq. 2.8).

We start with some additional notation: Let $\mathcal{R}$ denote a rectangle formed by the points

$$[-1/2, 1/2] \times [-i\delta, 0]\,,$$

where the parameter δ was introduced in the beginning of this subsection. For a unit vector $e \in \mathbb{Z}^3$, we will decompose $\mathbb{T}^3 \ni p = p \cdot e \oplus p^\perp$, where $p^\perp \in \mathbb{T}^2$. In what follows we will use the norm $\|\cdot\|_{\infty,\mathcal{R}}$ defined as

$$\|f\|_{\infty,\mathcal{R}} := \max_{e} \sup_{p\cdot e \in \mathcal{R},\ p^\perp \in \mathbb{T}^2} |f(p)|\,. \tag{2.34}$$

For u satisfying (2.5) and δ sufficiently small

$$\begin{aligned}
|\hat{u}(p)| &= \left| \sum_{x\in\mathbb{Z}^3} u(x) e^{-i2\pi x p} \right| \\
&= \left| \sum_{x\in\mathbb{Z}^3} u(x) e^{-i2\pi x \mathrm{Re}\, p} e^{2\pi x\cdot e \mathrm{Im}\, p\cdot e} \right| \\
&\leq |\hat{u}(\mathrm{Re}\, p)| + \left| \sum_{x\in\mathbb{Z}^3} u(x) e^{-i2\pi x \mathrm{Re}\, p} (e^{2\pi x\cdot e \mathrm{Im}\, p\cdot e} - 1) \right| \\
&\leq |\hat{u}(\mathrm{Re}\, p)| + \left| \sum_{x\in\mathbb{Z}^3} C|x| e^{-A|x|} 4\pi\delta \right| \\
&\leq |\hat{u}(\mathrm{Re}\, p)| + (4\pi)^2 C A^{-4} \delta,
\end{aligned}$$

so one has the following relation,

$$\|\hat{u}\|_{\infty,\mathcal{R}} \;\leq\; \|\hat{u}\|_\infty \,+\, (4\pi)^2 C A^{-4}\delta\,. \tag{2.35}$$

We will show that for a general value of l,

$$\mathcal{A}_{l,E}(x) \;\leq\; \|\hat{u}\|_{\infty,\mathcal{R}}^{2l} \cdot e^{-|x|\,\delta/\sqrt{3}}\; \hat{\mathcal{A}}_{l,E^*}(0)\,, \tag{2.36}$$

where

$$\begin{aligned}
\hat{\mathcal{A}}_{l,E^*}(0) \;:=\; \lambda^{2l} \int_{(\mathbb{T}^3)^{2l+2}} e^{i\alpha}\, \frac{dp_{l+1}}{e(p_{l+1})+E^*}\, \frac{dp_{2l+2}}{e(p_{2l+2})+E^*} \prod_{j\in\Upsilon_l} \frac{dp_j}{e(p_j)+E^*} \\
\times \sum_{\substack{\pi\in\Pi_l:\\ \pi=\pi_0}} \prod_{S_k\in\pi} c_{|S_k|}\, \delta\left(\sum_{i\in S_k} p_i - p_{i+1} \right),
\end{aligned} \tag{2.37}$$

with α defined in Lemma 2.2.3.

The expression $\hat{\mathcal{A}}_{l,E^*}(0)$ has been studied in Section 4 of [26]. It was shown there that

$$\hat{\mathcal{A}}_{l,E^*}(0) \;\leq\; (4l)!\, E^* \left(C \ln^9(E^*)\, \frac{\lambda^2}{\sqrt{E^*}} \right)^l. \tag{2.38}$$

Combining (2.36), (2.38) and (2.35), we obtain (2.29). Also, since A_0 was defined to be equal R_r in Lemma 2.3.1, we get $\hat{\mathcal{A}}_{0,E^*}(0) = (G_{E^*}(0,0))^2$. Equation (2.31) follows from the bound (2.68) on the free Green function.

To obtain relation (2.30) first note from Lemma 2.2.1:

$$\tilde{A}_N = A_N(H_r - E - i\epsilon) - A_{N-1}\sigma(E+i\epsilon)$$

So we get

$$\begin{aligned}\mathbb{E}\left|\tilde{A}_N(x,y)\right| &= \mathbb{E}\left|\sum_{z\in\mathbb{Z}^3}\left\{A_N(x,z)\cdot(H_r-E-i\epsilon)(z,y)-A_{N-1}(x,z)\cdot\sigma(z,y)\right\}\right| \\ &\le \sum_{z\in\mathbb{Z}^3}\left\{(\mathbb{E}\left|A_N(x,z)^2\right|)^{1/2}\left|(H_r-E-i\epsilon)(z,y)\right|+(\mathbb{E}\left|A_{N-1}(x,z)\right|^2)^{1/2}\left|\sigma(z,y)\right|\right\} \\ \le \sum_{z\in\mathbb{Z}^3,|z-y|\le 1}&(\mathbb{E}\left|A_{N-1}(x,z)\right|^2)^{1/2}+|\sigma(x,y)|\sum_{z\in\mathbb{Z}^3}\left((\mathbb{E}\left|A_N(x,z)\right|^2)^{1/2}+\mathbb{E}\left|A_{N-1}(x,z)\right|^2)^{1/2}\right) \\ &\le \tilde{C}\sqrt{(4N)!E^*}\left(C(E^*)\,\frac{\lambda^2}{\sqrt{E^*}}\right)^{N/2} e^{-\delta|x-y|/2}+C'\lambda^2\end{aligned}$$

where in the last step we used bound (2.29) and bound on σ from Appendix 2.5.2. Now provided both E^* and λ are sufficiently small, we arrive at relation (2.30).

To prove that (2.36) holds true let us choose for any given $x\in\mathbb{Z}^3$ the index $\gamma\in\{1,2,3\}$ such that

$$|x_\gamma| = \max_{i\in\{1,2,3\}}|x_i|\,. \tag{2.39}$$

Then $|x_\gamma|\ge|x|/\sqrt{3}$. In order to extract the exponential decay of $\mathcal{A}_{l,E}(x)$ we first perform the integration in the right hand side of (2.24) over the tree momenta, using (2.33).

Let us use the shorthand notation $\sum_\pi$ for a sum over all possible partitions in (2.24), c_π for a product of the corresponding c_{Sj}, r_π for the number of the delta functions containing the loop momentum w_1 in the π's partition, and s_π will denote the number of $\hat{u}$ terms involving w_1 after the integration of tree momentums.

Let $E(p)=e(p)-E-i\epsilon-\sigma(p,E+i\epsilon)$. We have

$$\begin{aligned}\mathcal{A}_{l,E}(x) \;=\; \lambda^{2l}\sum_\pi c_\pi\int dw_1\, e^{-i2\pi w_1\cdot x}\prod_{i=1}^{r_\pi}\frac{1}{E^\sharp(w_1+q_i)}\prod_{j=1}^{s_\pi}\hat{u}(w_1+Q_j) \\ \times\int \mathrm{e}^{-i2\pi w_2\cdot x}\prod_{t\in\Phi'}dw_t\prod_{i=r_\pi+1}^{2n+2}\frac{1}{E^\sharp(q_i)}\prod_{j=s_\pi+1}^{2n}\hat{u}(Q_j)\,,\end{aligned} \tag{2.40}$$

where $E^\sharp(p)$ stands for either $E(p)$ or $E^*(p)$, Φ' is a set of indices of loop momentum that does not include w_1, and q_i, Q_j are some linear combinations of the loop variables in Φ'.

Note now that

$$\int dw_1 \prod_{i=1}^{r_\pi} \frac{1}{E^\sharp(w_1+q_i)}\, e^{-i2\pi w_1\cdot x} \prod_{j=1}^{s_\pi} \hat{u}(w_1+Q_j)$$
$$= \int dw_1^\perp\, e^{-i2\pi(w_1\cdot x-(w_1\cdot e_\gamma)x_\gamma)}$$
$$\times \int_{-1/2}^{1/2} d(w_1\cdot e_\gamma) \prod_{i=1}^{r_\pi} \frac{1}{E^\sharp(w_1+q_i)}\, e^{-i2\pi(w_1\cdot e_\gamma)x_\gamma} \prod_{j=1}^{s_\pi} \hat{u}(w_1+Q_j)\,. \quad (2.41)$$

Without loss of generality, let us assume that $x_\gamma > 0$. The integrand as a function of $w_1\cdot e_\gamma$ is 1-periodic, analytic inside the rectangle $\mathcal{R}_- := \mathbb{C}_-\cap\mathcal{R}$ for sufficiently small E^*. Moreover, we have

$$\begin{aligned} \mathrm{Re}\, e(p-i\delta e_\gamma) &= e(p) - 2\sin^2(\pi p\cdot e_\gamma) + 2\mathrm{Re}\sin^2(\pi p\cdot e_\gamma - i\delta\pi) \\ &= e(p) + 2\sinh^2(\delta\pi)\left(\sin^2(\pi p\cdot e_\gamma) - \cos^2(\pi p\cdot e_\gamma)\right) \\ &\geq e(p) - 4\pi^2\delta^2 \end{aligned} \quad (2.42)$$

uniformly in $p\in\mathbb{T}^3$, provided δ is sufficiently small, where we have used the definition (1.4) and in the second equality we used

$$\sin(a+ib) \;=\; \sin a\cosh b + i\cos a\sinh b\,. \quad (2.43)$$

Combining this bound with (2.26), we get

$$|E(p-i\delta e_\gamma)| \;>\; e(p) \;+\; E^*\,, p\in\mathbb{T}^3\,. \quad (2.44)$$

Moreover, the periodicity of the integrand implies that the integrals over the vertical segments of $\mathcal{R}_-$ coincide:

$$\int_{-1/2}^{-1/2-i\delta} d(w_1\cdot e_\gamma) \prod_{i=1}^{r_\pi} \frac{1}{E^\sharp(w_1+q_i)}\, e^{-i2\pi x_\gamma\,(w_1\cdot e_\gamma)} \prod_{j=1}^{s_\pi} \hat{u}(w_1+Q_j)$$
$$= \int_{1/2}^{1/2-i\delta} d(w_1\cdot e_\gamma) \prod_{i=1}^{r_\pi} \frac{1}{E^\sharp(w_1+q_i)}\, e^{-i2\pi x_\gamma\,(w_1\cdot e_\gamma)} \prod_{j=1}^{s_\pi} \hat{u}(w_1+Q_j). \quad (2.45)$$

Therefore

$$\begin{aligned}
&\left| \int_{\mathbb{T}} d(w_1 \cdot e_\gamma) \prod_{i=1}^{r_\pi} \frac{1}{E^\sharp(w_1+q_i)} \, e^{-i2\pi x_\gamma (w_1 \cdot e_\gamma)} \prod_{j=1}^{s_\pi} \hat{u}(w_1+Q_j) \right| \\
&\qquad = \left| \int_{\mathbb{T}-i\delta} d(w_1 \cdot e_\gamma) \prod_{i=1}^{r_\pi} \frac{1}{E^\sharp(w_1+q_i)} \, e^{-i2\pi x_\gamma (w_1 \cdot e_\gamma)} \prod_{j=1}^{s_\pi} \hat{u}(w_1+Q_j) \right| \\
&\qquad\qquad \leq \ \|\hat{u}\|_{\infty,\mathcal{R}}^{s_\pi} \cdot e^{-x_\gamma \delta} \int_{\mathbb{T}} d(w_1 \cdot e_\gamma) \prod_{i=1}^{r_\pi} \left| \frac{1}{E\,(w_1+q_i-ie_\gamma\delta)} \right| \\
&\qquad\qquad\qquad \leq \ \|\hat{u}\|_{\infty,\mathcal{R}}^{s_\pi} \cdot e^{-|x|\,\delta/\sqrt{3}} \int_{\mathbb{T}} d(w_1 \cdot e_\gamma) \prod_{i=1}^{r_\pi} \frac{1}{e(w_1+q_i)+E^*} \,, \quad (2.46)
\end{aligned}$$

where in the last step we have used (2.44). Using the estimate (2.81), we also have

$$|E(p)| \ > \ e(w_1+q_i)+E^* \,, \quad p \in \mathbb{T}^3 \,.$$

Putting everything together on the right hand side of (2.40), we get the bound (2.36).

□

2.4 Localization at the bottom of the spectrum and Wegner estimate

Now we can proceed to prove Anderson localization (Theorem 2.1.1) at the bottom of the spectrum.

The initial volume estimate that enters into MSA requires us to get rid of the imaginary part ϵ of the energy, present in the formulation of Lemma 2.3.1. To this end, we will use the Wegner estimate below, that itself is an important ingredient of MSA. It will be established using the idea of F. Klopp [49]. While it has the correct (linear) dependence on the length of the interval I, the dependence on the volume of the estimate below is not optimal. The optimal, linear dependence on Λ for the continuum models with absolute continuous density ρ was developed in [39], but the trade-in is that the I-dependence in the Wegner estimate thereof is worse than ours. The derivation below has an advantage of being completely elementary and the estimate itself is sufficient for our purposes.

Theorem 2.4.1 (Wegner estimate for Liftshitz continuous densities)**.** *Let I be an open interval of energies such that*

$$D_I \ := \ \operatorname{dist}(I, \sigma(-\Delta/2)) \ > \ 0 \,.$$

Then we have

$$\mathbb{E}\ \mathrm{Tr}\, P_I(H_\omega^{\Lambda,\lambda}) \ \leq\ C\,|I|\,|\Lambda|^2\,(D_I)^{-1}\,, \tag{2.47}$$

where $H_\omega^{\Lambda,\lambda}$ denotes a natural restriction of H_ω^λ to $\Lambda \subset \mathbb{Z}^3$ and the constant C depends on J and K.

Proof of Theorem 2.1.1.

The proof assumes Theorem 2.4.1 which will be proven later in this section.

Let us denote by $H_\omega^{\Lambda,\lambda}$ the natural restriction of H_ω^λ to $\Lambda \subset \mathbb{Z}^3$, namely, $H_\omega^{\Lambda,\lambda}(i,j) = H_\omega^\lambda(i,j)$ if $(i,j) \in \Lambda \times \Lambda$ and $H_\omega^{\Lambda,\lambda}(i,j) = 0$ otherwise. Let $\Lambda^c := \mathbb{Z}^3 \setminus \Lambda$, and let $\partial^-\Lambda$ be the inner boundary of the set Λ. We define the decoupled Hamiltonian H_Λ to be

$$H_\Lambda = H_\omega^{\Lambda,\lambda} \oplus H_\omega^{\Lambda^c,\lambda}\,,$$

and $R_\Lambda(E)$ is the corresponding resolvent. Again for $L > 0$ and $x \in \mathbb{Z}^d$, $\Lambda_L(x) = \{y \in \mathbb{Z}^d : |x-y|_\infty \leq L\}$ the cube of side length $2L$. Our first objective is to derive the bound for $\mathbb{E}|R_{\Lambda_L(x)}(E+i\epsilon;x,w)|$, for $w \in \partial\Lambda$. To this end, we observe

$$\begin{aligned}
&\mathbb{E}|R_{\Lambda_L(x)}(E+i\epsilon;x,w)| \\
&\qquad \leq\ \mathbb{E}|R(E+i\epsilon;x,w)| \,+\, \mathbb{E}|R_{\Lambda_L(x)}(E+i\epsilon;x,w) \,-\, R(E+i\epsilon;x,w)| \\
&\qquad =\ \mathbb{E}|R(E+i\epsilon;x,w)| \,+\, \mathbb{E}|\big(R(H_\omega - H_{\Lambda_L(x)})\,R_{\Lambda_L(x)}\big)\,(x,w)| \\
&\qquad\qquad \leq\ \mathbb{E}|R(E+i\epsilon;x,w)| \\
&\qquad\qquad +\ \mathbb{E}\sum_{k\in\partial^-\Lambda_L^c(x)} |R(E+i\epsilon;x,k)|\,|\big(R_{\Lambda_L(x)}(H_\omega - H_{\Lambda_L(x)})\big)\,(k,w)|\,.
\end{aligned} \tag{2.48}$$

We can estimate

$$\sum_{k\in\partial\Lambda_L^c(x)} |\big(R_{\Lambda_L(x)}(H_\omega - H_{\Lambda_L(x)})\big)\,(k,w)| \ \leq\ \frac{C_0}{\epsilon}\,|\partial^-\Lambda| \ =\ C\,\frac{L^2}{\epsilon}\,, \tag{2.49}$$

hence

$$\mathbb{E}|R_{\Lambda_L(x)}(E+i\epsilon;x,w)| \ \leq\ C\,\frac{L^2}{\epsilon}\ \max_{k\in\partial\Lambda_L^c(x)}\ \mathbb{E}|R(E+i\epsilon;x,k)|\ . \tag{2.50}$$

On the other hand, for any $k \in \partial^-\Lambda_L^c(x)$, we have $\mathrm{dist}(x,k) = L+1$, and Lemma 2.3.1

ensures that

$$\begin{aligned}
\mathbb{E}|R(E+i\epsilon;x,k)| \;&\leq\; \sum_{n=0}^{N-1}\mathbb{E}|A_n(x,k)| \;+\; \sum_{z\in Z^3}\mathbb{E}|\tilde{A}_N(x,z)R(E+i\epsilon;z,k)| \\
&\leq\; \sum_{n=0}^{N-1}\Big\{\mathbb{E}|A_n^2(x,k)|\Big\}^{1/2} \;+\; \frac{1}{\epsilon}\sum_{z\in Z^3}\mathbb{E}|\tilde{A}_N(x,z)| \\
&\leq\; \sum_{n=0}^{N-1}\sqrt{(4n)!}\,\sqrt{E^*}\,\left(C(E^*)\,\frac{\lambda^2}{\sqrt{E^*}}\right)^{n/2} e^{-\delta\,|x-k|/2} \\
&\quad+\; \sum_{z\in Z^3}\frac{\sqrt{(4N)!}}{\epsilon}\,\left(C(E^*)\,\frac{\lambda^2}{\sqrt{E^*}}\right)^{N/2} e^{-\delta\,|x-z|/2} \\
&\leq\; e^{-\delta L/2}\sum_{n=0}^{N-1}\sqrt{E^*(4n)!}\,\left(C(E^*)\,\frac{\lambda^2}{\sqrt{E^*}}\right)^{n/2} \\
&\qquad\qquad+\; C\,\frac{\sqrt{(4N)!}}{\epsilon}\,\delta^{-3}\left(C(E^*)\,\frac{\lambda^2}{\sqrt{E^*}}\right)^{N/2} \qquad (2.51)
\end{aligned}$$

Choosing

$$(4N)^4 \;=\; \frac{\sqrt{E^*}}{C(E^*)\,\lambda^2}\,, \qquad (2.52)$$

one obtains, using the Stirling's approximation, that the summation over the index n is bounded by a constant and

$$(4N)!\left(\frac{C(E^*)\lambda^2}{\sqrt{E^*}}\right)^N \;\approx\; e^{-N}\,.$$

Hence, for such a value of N we have

$$\mathbb{E}|R(E+i\epsilon;x,k)| \;\leq\; C\,\left(e^{-\delta\,L/2}+\frac{e^{-N}}{\epsilon\,\delta^3}\right)\,. \qquad (2.53)$$

Combining this bound with (2.50), we obtain

$$\mathbb{E}|R_{\Lambda_L(x)}(E+i\epsilon;x,w)| \;\leq\; C\,\frac{L^2}{\epsilon}\left[e^{-\delta\,L/2}\;+\;\frac{e^{-N}}{\epsilon\,\delta^3}\right]\,. \qquad (2.54)$$

Let $I=[E-\epsilon^{1/4},E+\epsilon^{1/4}]$, and let

$$G(I) \;:=\; \big\{\omega\in\Omega:\;\sigma(H_{\Lambda_L(x)})\cap I=\emptyset\big\}\,.$$

For any $\omega\in G(I)$ we have by the first resolvent identity

$$\big|R_{\Lambda_L(x)}(E+i\epsilon;x,w)-R_{\Lambda_L(x)}(E;x,w)\big|\leq\epsilon^{1/2}\,.$$

Pairing this bound with (2.54) and using Chebyshev's inequality, we get that

$$\text{Prob}\left\{\omega \in G(I) :\ |R_{\Lambda_L(x)}(E;x,w)| \geq C\frac{L^2}{\epsilon^{5/4}}\left[e^{-\delta\, L/2} \,+\, \frac{e^{-N}}{\epsilon\,\delta^3}\right] \,+\, \epsilon^{1/4}\right\} \leq\ \epsilon^{1/4}\,. \quad (2.55)$$

The Wegner estimate (2.47) implies that

$$\text{Prob}\big\{\sigma(H_{\Lambda_L(x)}) \cap I \neq \emptyset\big\}\ \leq\ C\,|I|\ |\Lambda_L(x)|^2\,(D_I)^{-1}\ =\ C\,\epsilon^{1/4}\,(D_I)^{-1}\,L^6\,. \quad (2.56)$$

Combining (2.55) and (2.56) we arrive at

$$\text{Prob}\left\{|R_{\Lambda_L(x)}(E;x,w)| \geq C\frac{L^2}{\epsilon^{5/4}}\left[e^{-\delta\, L/2} \,+\, \frac{e^{-N}}{\epsilon\delta^3}\right] \,+\, \epsilon^{1/4}\right\} \leq\ C\epsilon^{1/4}\,(D_I)^{-1}\,L^6\,. \quad (2.57)$$

We are now in position to set the values for the various parameters in the above formula, in terms of the single parameter λ. We first note that since $E \leq E_0 - \lambda^{4-\nu}$ with $0 < \nu < 1$ and E_0 defined in (2.6), it is allowed to choose $E^* = \lambda^{4-\nu}/2$. It then follows from (2.32) and (2.52) that $N \sim \lambda^{-B'\nu}$ with $0 < B' < 1/4$, for λ small enough. Next, the parameter δ originating from 2.3.1 satisfies $\delta \sim \lambda^{2-\nu/2}$ for λ small enough. We finally choose $L = \lambda^{-2}$ and $\epsilon = e^{-5\lambda^{-B'\nu/2}}$. Plugging it all into (2.57) we obtain that for the small values of λ the following initial volume estimate holds true:

$$\text{Prob}\left\{|R_{\Lambda_{\lambda^{-2}}(x)}(E;x,w)| \geq e^{-\lambda^{-B'\nu/2}}\right\}\ \leq\ e^{-\lambda^{-B'\nu/2}}\,. \quad (2.58)$$

The initial volume estimate (2.58) together with the Wegner estimate (2.56) provide the necessary input for MSA for small λ, and the result follows from say Theorem 2.4 of [36].

□

Proof of Theorem 2.4.1. We first observe that for any random quantity F_ω that depends on the random variables ω_i, with $i \in \Lambda$, we have for any δ

$$\mathbb{E}F_\omega\ =\ \int F_\omega \prod_{i\in\Lambda}\rho(\omega_i)d\omega_i\ =\ \frac{1}{2\delta}\int_{1-\delta}^{1+\delta} v^{|\Lambda|}dv \int F_{v\hat{\omega}} \prod_{i\in\Lambda}\rho(v\hat{\omega}_i)d\hat{\omega}_i\,. \quad (2.59)$$

So, in order to evaluate

$$\mathbb{E}\ Im\ \left(H_\omega^{\Lambda,\lambda} - E - i\eta\right)^{-1}\,,$$

we can first integrate over the fictitious random variable v. To this end, observe that $H_\omega^{\Lambda,\lambda} = \Delta_\Lambda + v\lambda V_{\hat{\omega}}$, hence

$$Im\ \left(H_\omega^{\Lambda,\lambda} - E - i\eta\right)^{-1}\ =\ \frac{\eta}{v^2}\ \left((v^{-1}A + V_{\hat{\omega}})^2 + v^{-2}\eta^2\right)^{-1}\,,$$

where the operator A is equal to $\Delta_\Lambda - E > E^*$ for all $E \in I$. Choosing $\delta = |\Lambda|^{-1}$ and using the positivity of the expression above for $\eta > 0$, we can estimate

$$\begin{aligned}\mathbb{E}\ \mathrm{Tr}\ Im\ \left(H_\omega^{\Lambda,\lambda} - E - i\eta\right)^{-1} \\ \leq\ \frac{e}{2\delta}\int_{1-\delta}^{1+\delta} dv \int \frac{\eta}{v^2}\ \mathrm{Tr}\ \left((v^{-1}A + V_{\hat\omega})^2 + (\eta/2)^2\right)^{-1} \prod_{i\in\Lambda}\rho(v\hat\omega_i)d\hat\omega_i\,. \quad (2.60)\end{aligned}$$

Using Assumption (2.4) we can bound the right hand side as

$$\begin{aligned}\frac{C}{\delta}\int \prod_{i\in\Lambda}\left(\rho(\hat\omega_i)\ +\ K\delta\,\mathbf{1}_{J'}(\hat\omega_i)\right)d\hat\omega_i \int_{1-\delta}^{1+\delta} dv\frac{\eta}{v^2}\ \mathrm{Tr}\ \left((v^{-1}A + V_{\hat\omega})^2 + (\eta/2)^2\right)^{-1} \\ \leq\ \frac{C\eta}{\delta}\int \prod_{i\in\Lambda}\left(\rho(\hat\omega_i)\ +\ K\delta\,\mathbf{1}_{J'}(\hat\omega_i)\right)d\hat\omega_i \int_{-\infty}^{\infty} du\ \mathrm{Tr}\ \left((uA + V_{\hat\omega})^2 + (\eta/2)^2\right)^{-1}\,, \quad (2.61)\end{aligned}$$

where $J' = (1+\delta)J$. We now in position to estimate the integral over the u variable in the above expression. To this end, we write

$$\begin{aligned}(uA + V_{\hat\omega})^2 + (\eta/2)^2 \\ =\ A^{1/2}\left((u + A^{-1/2}V_{\hat\omega}A^{-1/2})A(u + A^{-1/2}V_{\hat\omega}A^{-1/2}) + (\eta/2)^2A^{-1}\right)A^{1/2} \\ \geq\ A^{1/2}\left(E^*(u + A^{-1/2}V_{\hat\omega}A^{-1/2})^2 + \frac{\eta^2}{4\|A\|}\right)A^{1/2}\,. \quad (2.62)\end{aligned}$$

Since $\mathrm{Tr}\, DB^2D = \mathrm{Tr}\, BD^2B$ for a pair of the hermitian matrices B, D, we infer

$$\begin{aligned}\mathrm{Tr}\left((uA + V_{\hat\omega})^2 + (\eta/2)^2\right)^{-1} \\ \leq\ \mathrm{Tr}\, A^{-1/2}\left(E^*(u + A^{-1/2}V_{\hat\omega}A^{-1/2})^2 + \frac{\eta^2}{4\|A\|}\right)^{-1}A^{-1/2} \\ =\ \mathrm{Tr}\left(E^*(u + A^{-1/2}V_{\hat\omega}A^{-1/2})^2 + \frac{\eta^2}{4\|A\|}\right)^{-1/2}A^{-1} \\ \times\ \left(E^*(u + A^{-1/2}V_{\hat\omega}A^{-1/2})^2 + \frac{\eta^2}{4\|A\|}\right)^{-1/2} \\ \leq\ \left\|A^{-1}\right\|\ \mathrm{Tr}\left(E^*(u + A^{-1/2}V_{\hat\omega}A^{-1/2})^2 + \frac{\eta^2}{4\|A\|}\right)^{-1}\,. \quad (2.63)\end{aligned}$$

Using the identity

$$\int_{\mathbb{R}} du\ \left((u+D)^2\,I_n\ +\ b^2\right)^{-1}\ =\ \pi\, b^{-1}\, I_n\,,$$

for any hermitian matrix D and any positive b, we obtain the bound

$$\int_{-\infty}^{\infty} du\ \mathrm{Tr}\left((uA + V_{\hat\omega})^2 + (\eta/2)^2\right)^{-1}\ \leq\ \left\|A^{-1}\right\|\ \pi\,\frac{2\,\|A\|^{1/2}}{(E^*)^{1/2}\,\eta}\ |\Lambda|\,. \quad (2.64)$$

Using $\|A^{-1}\| \leq (E^*)^{-1}$, $\|A\| < 7$ (which hold for $E^* < 1$), and the latter bound to estimate the right hand side of (2.61), we arrive to the estimate

$$\mathbb{E}\ \mathrm{Tr}\ Im\ \left(H_\omega^{\Lambda,\lambda} - E - i\eta\right)^{-1} \leq\ \frac{C}{\delta}\,(E^*)^{-3/2}\ |\Lambda| \int \prod_{i\in\Lambda} \left(\rho(\hat{\omega}_i)\ +\ K\delta\,\mathbf{1}_{J'}(\hat{\omega}_i)\right) d\hat{\omega}_i\ =\ \tilde{C}|\Lambda|^2\,(E^*)^{-3/2}\,, \quad (2.65)$$

uniformly in η. Using

$$P_I(H_\omega^\Lambda)\ =\ \int_I dE\ \lim_{\eta\downarrow 0} Im\ \left(H_\omega^{\Lambda,\lambda} - E - i\eta\right)^{-1} \quad (2.66)$$

for the open interval I, we finally arrive to the estimate

$$\mathbb{E}\ \mathrm{Tr}\, P_I(H_\omega^{\Lambda,\lambda})\ \leq\ C\,|I|\ |\Lambda|^2\,(E^*)^{-3/2}\,. \quad (2.67)$$

□

2.5 appendix

2.5.1 Bounds on the free Green function

The free Green function $G_E(x,y)$ was defined in (2.27). We have

Lemma 2.5.1. *Define the function $\psi_\alpha \in l_2(\mathbb{Z}_+)$ as*

$$\psi_\alpha(r)\ =\ e^{-r\frac{\sqrt{-E}}{\alpha}}\ \max\left((-E)^{(d-2)/2}\,,\,(1+r)^{(2-d)}\right)\,.$$

Then for $d \geq 3$ and $-1 < E < 0$ we have

$$0\ <\ G_E(x,y)\ <\ C_d\ \psi_{3d}(|x-y|)\,, \quad (2.68)$$

for all $x, y \in \mathbb{Z}^d$.

Remark 4. A similar statement is known to hold on $\mathbb{R}^d$, [65]. We are not aware of its lattice version in the existing literature. The positivity of $G(x,y)$ on the lattice is well known, so it is an upper bound we are after here.

Proof.

In what follows, we will use the following properties of the function ψ for $d \geq 3$ and E^* sufficiently small:

(a)
$$\|\psi_\alpha\|_\infty \;=\; 1\,;$$

(b)
$$\sum_{x\in\mathbb{Z}^d} \psi_\alpha(|x-y|) \;=\; \frac{C_d\alpha}{-E} \text{ for any } y\in\mathbb{Z}^d\,;$$

(c)
$$\psi_\alpha(|r\pm b|) \;\le\; C(\Theta)\,\psi_\alpha(r) \text{ for } 0<b<\operatorname{diam}(\Theta)\,;$$

(d)
$$\prod_{i=1}^{2n+1} \psi_\alpha(|x_{i-1}-x_i|) \;\le e^{-|x_{2n+1}-x_0|\frac{\sqrt{-E}}{2\alpha}} \prod_{i=1}^{2n+1} \psi_{\alpha/2}(|x_{i-1}-x_i|)\,.$$

Suppressing the subscript E in the free Green function, we have

$$G(x,y) \;=\; \int_{\mathbb{T}^d} e^{i2\pi(x-y)p}\frac{d^dp}{e(p)-E} \;=\; \int_{\mathbb{T}^d} e^{i2\pi(x-y)p}\frac{d^dp}{e(p)-E}\,.$$

Let $w=x-y$. For any given $w\in\mathbb{Z}^d$ let us choose $\gamma\in\{1,\dots,d\}$ so that

$$|w\cdot e_\gamma| = \max_{i\in\{1,\dots,d\}} |w\cdot e_i|\,. \tag{2.69}$$

Then

$$|w\cdot e_\gamma| \ge |w|/\sqrt{d}\,. \tag{2.70}$$

Note that

$$\int dp\,\frac{1}{e(p)-E}\,e^{-i2\pi p\cdot w} \;=\; \int dq\,e^{-i2\pi q\cdot w}\int_{-1/2}^{1/2} d(p\cdot e_\gamma)\,\frac{1}{e(p)-E}\,e^{-i2\pi(p\cdot e_\gamma w\cdot e_\gamma)}\,, \tag{2.71}$$

where q stands for the $d-1$ dimensional vector obtained from p by removing its γ component (for $d=1$ the argument below becomes completely straightforward, so we will only consider $d\ge 2$). Without loss of generality, let us assume that $w\cdot e_\gamma>0$. Let

$$\hat e(q) = 2\sum_{\alpha\neq\gamma}\sin^2(\pi p\cdot e_\alpha)\,.$$

It is easy to check that the integrand as a function of $p\cdot e_\gamma$ is 1-periodic, analytic inside the rectangle formed by the points

$$\{-1/2;\; -1/2+i\sqrt{\frac{\hat e(q)-E}{6d}};\; 1/2+i\sqrt{\frac{\hat e(q)-E}{6d}};\; 1/2\}$$

for a sufficiently small value of $-E > 0$: Indeed, using $\sin(a+ib) = \sin a \cosh b + i \cos a \sinh b$ one can check that for any $-1 < E < 0$ and ϵ satisfying

$$0 \le \epsilon \le \sqrt{\frac{\hat{e}(q) - E}{6d}}$$

we have

$$\operatorname{Re} e(p + i\epsilon e_\gamma) - E \ge (e(p) - E)/2\,,$$

uniformly in q. Moreover, the periodicity implies that the integrals over the vertical segments coincide:

$$\int_{-1/2}^{-1/2+i\sqrt{\frac{e(q)-E}{6d}}} d(p\cdot e_\gamma) \frac{1}{e(p)-E}\, e^{-i2\pi(p\cdot e_\gamma w\cdot e_\gamma)} = \int_{1/2}^{1/2+i\sqrt{\frac{e(q)-E}{6d}}} d(p\cdot e_\gamma)\, \frac{1}{e(p)-E}\, e^{-i2\pi(p\cdot e_\gamma w\cdot e_\gamma)}\,. \quad (2.72)$$

Therefore

$$\begin{aligned}\left|\int_{-1/2}^{1/2} d(p\cdot e_\gamma)\, \frac{1}{e(p)-E}\, e^{-i2\pi(p\cdot e_\gamma w\cdot e_\gamma)}\right| &= \left|\int_{-1/2+i\sqrt{\frac{e(q)-E}{6d}}}^{1/2+i\sqrt{\frac{e(q)-E}{6d}}} d(p\cdot e_\gamma)\, \frac{1}{e(p)-E}\, e^{-i2\pi(p\cdot e_\gamma w\cdot e_\gamma)}\right| \\ &\le 2\, e^{-w\cdot e_\gamma \sqrt{\frac{e(q)-E}{6d}}} \int_{-1/2}^{1/2} d(p\cdot e_\gamma)\, \frac{1}{e(p)-E} \\ &\le 4\, e^{-|w|\frac{\sqrt{e(q)-E}}{3d}}\, \frac{1}{\sqrt{e(q)-E}}\,, \quad (2.73)\end{aligned}$$

where in the last step we used (2.70). We can consequently estimate the right hand side of (2.71) by

$$4 \int dq\, e^{-|w|\frac{\sqrt{e(q)-E}}{3d}}\, \frac{1}{\sqrt{e(q)-E}}\,.$$

To estimate the latter integral, we split $\mathbb{T}^{d-1}$ into $B := \{q \in \mathbb{T}^{d-1} : \ e(q) \le -E\}$ and $\sim B := \mathbb{T}^{d-1} \setminus B$. Then

$$\begin{aligned}\int_B dq\, e^{-|w|\frac{\sqrt{e(q)-E}}{3d}}\, \frac{1}{\sqrt{e(q)-E}} &\le \int_B dq\, e^{-|w|\frac{\sqrt{-E}}{3d}}\, \frac{1}{\sqrt{-E}} \\ &\le C_d\, e^{-|w|\frac{\sqrt{-E}}{3d}}\, (-E)^{(d-2)/2}\,, \quad (2.74)\end{aligned}$$

and

$$\int_{\sim B} dq\, e^{-|w|\frac{\sqrt{e(q)-E}}{3d}}\, \frac{1}{\sqrt{e(q)-E}} \;\leq\; \int_{\sim B} dq\, e^{-|w|\frac{\sqrt{e(q)}}{3d}}\, \frac{1}{\sqrt{e(q)}}$$
$$\leq\; \int_{\sim B} dq\, e^{-|w|\frac{2}{3d}\sqrt{2q^2}}\, \frac{\pi}{2\sqrt{2q^2}}$$
$$\leq\; C_d\, e^{-|w|\frac{2\sqrt{2-E}}{3d}} \sum_{k=0}^{d-2} \frac{(d-2)!}{k!} \frac{(-E)^k}{|w|^{d-k-1}}\,, \quad (2.75)$$

for $d \geq 2$, and where in the penultimate step we have used Jordan's inequality. Summing up (2.74) and (2.75), we arrive to (2.68).

□

2.5.2 Properties of the self energy (2.8)

In this section we establish the existence, periodicity, and analyticity of the self energy operator $\sigma(p, E+i\epsilon)$ introduced in (2.8). We will use the following inequalities (that can be deduced from [44]):

$$\int_{\mathbb{T}^3} d^3q\, \frac{1}{e(q)} < 2\,, \quad \int_{\mathbb{T}^3} d^3q\, \frac{1}{(e(q)+\epsilon^2)^2} < \frac{1}{\epsilon}\,. \quad (2.76)$$

To prove the existence, we introduce the space

$$L(\mathbb{T}^3) \;=\; \{f \,:\, \mathbb{T}^3 \to \mathbb{C} \,\big|\, \|f\|_\infty < \infty\,, f \;\text{ is real analytic}\}\,.$$

We define a map $T_\epsilon : L(\mathbb{T}^3) \to L(\mathbb{T}^3)$ pointwise as

$$(T_\epsilon f)(p) = \lambda^2 \int_{\mathbb{T}^3} d^3q\, \frac{|\hat{u}(p-q)|^2}{e(q)-E-i\epsilon-f(q)}\,. \quad (2.77)$$

If we consider $\beta = 2\lambda^2\|\hat{u}\|_\infty^2$, and $E \leq -2\lambda^2\|\hat{u}\|_\infty^2$, then we have $T_\epsilon B_\beta(0) \subset B_\beta(0)$, where $B_\beta(0)$ is a ball (in $\|\cdot\|_\infty$ topology) of radius β centered at the origin. Indeed, for $f \in B_\beta(0)$,

$$\lambda^2 \left| \int_{\mathbb{T}^3} d^3q\, \frac{|\hat{u}(p-q)|^2}{e(q)-E-i\epsilon-f(q)} \right| \leq \lambda^2 \int_{\mathbb{T}^3} d^3q\, \frac{\|\hat{u}\|_\infty^2}{e(q)} < 2\lambda^2\|\hat{u}\|_\infty^2\,,$$

where we have used (2.76) in the last step.

Consider further $E \leq -2\lambda^2\|\hat{u}\|_\infty^2 - 2\lambda^4\|\hat{u}\|_\infty^4$, Then T_ϵ is a contraction on $B_\beta(0)$. Indeed, let $f, g \in B_\beta(0)$, then

$$|(T_\epsilon f)(p) - (T_\epsilon g)(p)| \;\leq \lambda^2 \int_{\mathbb{T}^3} d^3q\, \frac{|\hat{u}(p-q)|^2\, |f(q)-g(q)|}{|e(q)-E-i\epsilon-f(q)|\, |e(q)-E-i\epsilon-g(q)|}$$
$$\leq \lambda^2\|f-g\|_\infty \int_{\mathbb{T}^3} d^3q\, \frac{\|\hat{u}\|_\infty^2}{(e(q)+2\|\hat{u}\|_\infty^4\lambda^4)^2} \;\leq \frac{1}{\sqrt{2}}\|f-g\|_\infty\,, \quad (2.78)$$

where we have used (2.76) in the last step. Hence by the Banach fixed point theorem, the self consistent equation (2.8) has a single valued solution $\sigma(p, E + i\epsilon)$ for all $p \in \mathbb{T}^3$ and all

$$E < E_0 := -2\lambda^2 \|\hat{u}\|_\infty^2 - 2\lambda^4 \|\hat{u}\|_\infty^4 .$$

The function $\sigma(p, E + i\epsilon)$ satisfies

$$\|\sigma\|_\infty \;\leq\; 2\lambda^2 \|\hat{u}\|_\infty^2 . \tag{2.79}$$

Next we establish 1-periodicity of the above solution (in the real space). To this end, we note that since $\hat{u}(p-q) = \sum_{n\in\mathbb{Z}^3} u(n) e^{2\pi i (p-q)n}$, we have

$$|\hat{u}(p-q)|^2 = \sum_{m,n\in\mathbb{Z}^3} u(m)u(n) e^{2\pi i (p-q)(n-m)} .$$

Hence

$$\lambda^2 \int_{\mathbb{T}^3} d^3q \, \frac{|\hat{u}(p-q)|^2}{e(q) - E - i\epsilon - f(q)} = \lambda^2 \sum_{m,n\in\mathbb{Z}^3} u(m)u(n) e^{2\pi i p(n-m)} \int_{\mathbb{T}^3} d^3q \, \frac{e^{2\pi i q(m-n)}}{e(q) - E - i\epsilon - f(q)} , \tag{2.80}$$

and periodicity of $\sigma(p, E + i\epsilon)$ follows from the periodicity of $e^{2\pi i p(n-m)}$.

Finally, we show analyticity. Fix a unit vector $e \in \mathbb{Z}^3$, and let $p_e := p \cdot e$, $n_e := n \cdot e$ for $n \in \mathbb{Z}^3$. Using (2.76) one can readily check that

$$\left\| \frac{d^k \sigma(p, E + i\epsilon)}{d_{p_e}^k} \right\|_\infty \;\leq\; 2\lambda^2 \sum_{m,n\in\mathbb{Z}^3} \left| u(m)u(n)(2\pi)^k (n_e - m_e)^k \right| \;\leq\; C\, \lambda^2 A^{-k+3} k! ,$$

for all $p_e \in \mathbb{T}$, and where A is given by (2.5), and C is some generic constant. This implies that $\sigma(p, E + i\epsilon)$ is real analytic in p_e variable and admits the complex analytic continuation to the rectangle $\mathcal{R}$ introduced in the paragraph followed by (2.34). It follows from (2.76) that we also have in this energy interval the bound

$$\|\sigma\|_{\infty,\mathcal{R}} \;\leq\; 2\lambda^2 \, \|\hat{u}\|_{\infty,\mathcal{R}}^2 , \tag{2.81}$$

with the norm $\|\cdot\|_{\infty,\mathcal{R}}$ defined in (2.34).

2.5.3 Dipole single site potential

Here we consider a special case of the single site potential u_d defined in (2.9) Let T_ϵ be the same map as the one defined in (2.77). Then $|\hat{u}(p)|^2 = 4\sin^2(\pi p \cdot e_1)$, and for the even

function f we have

$$(T_\epsilon f)(p) \;=\; 4\lambda^2 \sin^2(\pi p\cdot e_1)\int_{\mathbb{T}^3} d^3q\,\frac{\cos(2\pi q\cdot e_1)}{e(q)-E-i\epsilon-f(q)} \\ +\;4\lambda^2\int_{\mathbb{T}^3} d^3q\,\frac{\sin^2(\pi q\cdot e_1)}{e(q)-E-i\epsilon-f(q)}\,. \quad (2.82)$$

We will consider the energies E that satisfy

$$E \;<\; -(1+\lambda)\lambda^2\,.$$

The subspace G of $L^\infty(\mathbb{T}^3)$ consisting of the functions $f(p)=A+B\sin^2(\pi p\cdot e_1)$ is clearly invariant under the map T_ϵ. Let G' denote a closed subset of G' characterized by $|A|\le\lambda^2$, $|B|\le 14\lambda^2$. We then have $T_\epsilon G'\subset G'$. Indeed, for $f\in G'$, we can estimate the two terms on the right hand side of (2.82) using two bounds below, that hold for λ sufficiently small:

$$\int_{\mathbb{T}^3} d^3q\,\frac{|\cos(2\pi q\cdot e_1)|}{|e(q)-E-i\epsilon-f(q)|} \qquad < \qquad \int_{\mathbb{T}^3} d^3q\,\frac{1}{(1-|B|)e(q)} \qquad < \qquad \frac{7}{2}\,, \quad (2.83)$$

where in the penultimate step we have used the symmetry of the integral with respect to spatial directions $\{1,2,3\}$ and in the last step we have used (2.76). The second estimate we need is

$$\int_{\mathbb{T}^3} d^3q\,\frac{2\sin^2(\pi q\cdot e_1)}{|e(q)-E-i\epsilon-f(q)|} \;<\; \int_{\mathbb{T}^3} d^3q\,\frac{2\sin^2(\pi q\cdot e_1)}{(1-|B|)e(q)} \;=\; \frac{1}{3(1-|B|)} \;<\; \frac{1}{2}\,. \quad (2.84)$$

Let $(T_\epsilon f)(p)=C+D\sin^2(\pi p\cdot e_1)$, the above two bounds give

$$C\le\lambda^2,\quad D\le 14\lambda^2\,, \quad (2.85)$$

hence $T_\epsilon f\in G'$. Since G' is a compact convex set, one can use Brouwer's fixed point theorem to conclude the existence of the fixed point (in fact one can use this technique to show the existence of the fixed point for *all* negative values of E). However, we also need a uniqueness of the fixed point, so we proceed to prove that T_ϵ is a contraction on G'. To this end, let us introduce a norm on G:

$$\|f\|_G \;=\; |A| \;+\; \lambda|B|\,, \qquad \text{for } f=A+B\sin^2(\pi p\cdot e_1)\,.$$

Let $f=A+B\sin^2(\pi p\cdot e_1), g=C+D\sin^2(\pi p\cdot e_1)\in G'$, then the straightforward computation similar to the one done in (2.78) gives

$$\|(T_\epsilon f)(p)-(T_\epsilon g)(p)\|_G \\ \le\; 4\lambda^2\int_{\mathbb{T}^3} d^3q\,\frac{(|A-C|+|B-D|)\sin^2(\pi q\cdot e_1)}{((1-|B|)e(q)+\lambda^3)\,((1-|D|)e(q)+\lambda^3)} \\ +\;4\lambda^3\int_{\mathbb{T}^3} d^3q\,\frac{|A-C|+|B-D|\sin^2(\pi q\cdot e_1)}{((1-|B|)e(q)+\lambda^3)\,((1-|D|)e(q)+\lambda^3)} \\ <\; 20\lambda^2|B-D|\;+\;5\lambda^{3/2}|A-C| \;<\; 20\lambda\|f-g\|_G\,, \quad (2.86)$$

for λ small enough. We have used (2.76) in the penultimate step. Hence by Banach fixed point theorem, the self consistent equation (2.8) has a single valued solution $\sigma(p, E+i\epsilon)$ for all $p \in \mathbb{T}^3$ and all

$$E \;<\; E_d \;:=\; -(1+\lambda)\lambda^2\,.$$

Since $\sigma \in G'$ we have

$$\sigma(p, E+i\epsilon) \;=\; A + B\sin^2(\pi p\cdot e_1)\,; \quad |A| \;\le\; \lambda^2\,,\; |B| \;\le\; 14\;\lambda^2\,. \tag{2.87}$$

It follows from the functional form of $\sigma(p, E+i\epsilon)$ that for any unit vector $e \in \mathbb{Z}^3$ the function σ is 1-periodic, analytic in $p_e := p\cdot e$ (in fact it is a constant unless $e = e_1$). Let E_d^* be a parameter that satisfies $0 < E_d^* < E_d - E$ and let

$$\delta \;:=\; \sqrt{(E_d - E - E_d^*)/2}\,.$$

Then using (2.43) and (2.87) we deduce that for an arbitrary $p \in \mathbb{T}^3$ we have

$$Re\,(e(p+i\delta e) - E - i\epsilon - \sigma(p+i\delta e, E+i\epsilon)) \;>\; (1-5\lambda^2)\,(e(p)+E_d^*)\;. \tag{2.88}$$

Proof of Proposition 2.1.2.

Let $\Lambda : [-L, L]^3 \cap \mathbb{Z}^3$, $\Lambda_+ : [-L-1, L+1]\times[-L, L]^2 \cap \mathbb{Z}^3$ and let $\Omega_\Lambda := \times_{k\in\Lambda_+}\mathbb{R}$. By the standard arguments (c.f. the discussion in Section 6 of [46]) it suffices to find a configuration $\omega \in \Omega_\Lambda$, for which $\min\sigma(H_\omega^\Lambda) < -2\lambda^2 + O(\lambda^3) + o(1)$. Here $o(1)$ is taken with respect to the L variable. We choose the following configuration of ω:

$$\omega(i) \;=\; \begin{cases} -1 & i\cdot e_1 \ge 0, i\cdot e_2 = 0, i\cdot e_3 = 0 \\ 1 & i\cdot e_1 \le -1, i\cdot e_2 = 0, i\cdot e_3 = 0\;. \\ 0 & \text{otherwise} \end{cases} \tag{2.89}$$

With this choice of ω, we have for $x \in \Lambda$, $V_\omega^\Lambda(x) = -2\lambda$ for $x\cdot e_1 = 0$ and $V_\omega^\Lambda(x) = 0$ otherwise. Clearly, the bottom of the spectrum of H_ω^Λ converges, in the limit $L\to\infty$, to $\inf\sigma(\hat{H})$, where the latter operator acts on the whole $\mathbb{Z}^3$ as

$$\hat{H} \;=\; -\frac{\Delta}{2} + \hat{V}\,,$$

with

$$\hat{V}(x) = -2\lambda \text{ for } x\cdot e_1 = 0 \text{ and } \hat{V}(x) = 0 \text{ otherwise}\,.$$

Readily, $\inf\sigma(\hat{H}) \le \min\sigma(\tilde{H})$, where $\tilde{H}$ is a one dimensional restriction of $\hat{H}$ to the e_1 direction. However, $\tilde{H}$ is a rank one perturbation of the free Laplacian. It follows from the rank one perturbation theory that $E_m := \min\sigma(\tilde{H})$ is given by the solution of the equation

$$\frac{1}{2\lambda} \;=\; G(E_m; \delta_0, \delta_0)\,,$$

where G is a free one dimensional Green function. Using the Fourier transform, the above equation can be rewritten as

$$\frac{1}{2\lambda} \;=\; \int_{\mathbb{T}} \frac{dq}{2\sin^2(\pi q) - E_m}\,.$$

Finally, since

$$\int_{\mathbb{T}} \frac{dq}{2\sin^2(\pi q) - E_m} \;=\; \int_{-\infty}^{\infty} \frac{dq}{2\pi^2 q^2 - E_m} \;+\; O(1) \;=\; \frac{1}{\sqrt{-2E_m}} \;+\; O(1)$$

which holds for $E_m < 0$, we obtain

$$E_m \;=\; -2\lambda^2 + O(\lambda^3)\,.$$

The rest of the argument coincides with Theorem 2.1.1. □

Chapter 3

Adiabatic quantum computation for low-rank matrices

3.1 Bounds on the running time in Hamiltonian–based quantum computation

In a mathematical formulation of AQC, one is interested in finding the ground state of a given problem Hamiltonian H_F, in the shortest possible time. To this end, we consider a pair of hermitian $N \times N$ matrices $H_{I,F}$, and will assume that $N \gg 1$. Let $H(s)$ be the interpolating Hamiltonian

$$H(s) := (1 - f(s))H_I + f(s)H_F\,, \tag{3.1}$$

where f is a monotone function on $[0, 1]$ satisfying $f(0) = 0$, $f(1) = 1$. The idea of AQC is to prepare the initial state of the system $\psi(0)$ in a ground state ψ_I of the Hamiltonian H_I, and let the system evolve according to the (scaled) Schrödinger equation:

$$i\dot{\psi}_\tau(s) \;=\; \tau H(s)\psi_\tau(s)\,, \quad \psi_\tau(0) \;=\; \psi_I\,. \tag{3.2}$$

The adiabatic theorem (AT) of quantum mechanics ensures that under certain conditions (see theorem 3.3.1 below for details) the evolution $\psi_\tau(1)$ of the initial state stays close to a ground state of the problem Hamiltonian H_F. For AQC to be efficient, the running (*i.e.* physical) time τ in (3.2) must be much smaller than N. One then can ask what choice of the initial Hamiltonian H_I and the parametrization $f(s)$ minimizes τ, and what the optimal value of τ is.

One of the parameters that enters into the upper bound for τ in the standard AT is the minimal value g of the spectral gap $g(s)$ between the ground state energy of $H(s)$ and the rest of its spectrum. Consequently, the traditional approach [33] to AQC involves the

estimation of g. Excluding a very short list of interesting situations for which g can be explicitly evaluated (compilation of such examples can be found in [22]), it appears to be a hard problem. In some instances, one can get an idea of what size g could be by using the first-order perturbation theory [69]. In subsection 3.4, we present rigorous bounds on the size of the gap for the problem at hand, albeit we don't use them explicitly in our study of AQC.

All the results presented here, *e.g.*, the rigorous upper and lower bounds on the optimal running time τ and the size of the spectral gap, apply to a particular class of problem Hamiltonians satisfying the following assumption.

Assumption 2. The problem Hamiltonian is of the small rank:

$$Rank(H_F) := m \ll N\,.$$

This hypothesis is fulfilled in particular for the generalized unstructured search (GUS) problem, see *e.g.* [15]. Since we are interested in the dynamical evolution of the initial state for which shifting the energy results in the overall dynamical phase factor, the above assumption is equivalent to the following condition: Let V denote the largest eigenspace of H_F. Then we require that $N - \dim V \ll N$.

It turns out that for such H_F one can circumvent the standard AT, avoiding the direct estimation of g. We will also see that the (nearly) optimal parametrization $f(s)$ is in fact non adiabatic.

To formulate the results, we need to introduce some notation first: Let $\{E_n^i\}_{n=1}^N$ ($\{E_n^f\}_{n=1}^N$) be a set of distinct eigenvalues of H_I (respectively H_F), enumerated in the ascending order. It is allowed to the corresponding eigenvalues to be degenerate. In what follows, we will denote by P_I (P_F) the eigenprojection of H_I (H_F) onto $E_I := E_1^i$ ($E_F := E_1^f$), and by Q_I (Q_F) the orthogonal projection onto the range of H_I (H_F). To AQC to be meanigful in our context we have to impose $E_I \neq 0$. In the typical setup, $E_I = -1$.

Before stating the results, let us note that for AQC to work, it suffices to ensure that $\psi_\tau(1)$ has just the non trivial overlap with the range of P_F, which we will encode in the requirement $\|P_F\psi_\tau(1)\| \geq \gamma$ for a "reasonable" γ. Indeed, like many quantum algorithms, the AQC algorithm is probabilistic in the sense that it gives the correct answer with the probability γ^2. The probability of failure can be decreased to the desired value (namely $O(1/N)$) by repeating the algorithm $\frac{\ln N}{\gamma^2}$ times. We set $\gamma = 1/5$ throughout this paper. Another issue that we want to settle is normalization of $H(s)$. To that end, we will calibrate $H_{I,F}$ as $\|H_I\| = \|H_F\| = 1$. Note that without loss of generality we can assume that $E_F < 0$ (since otherwise we can interpolate $-H_I$ and $-H_F$ which only changes the solution ψ_τ of (3.2) into $\bar{\psi}_\tau$). We now introduce some parameters in order to formulate our results. Namely, let $\delta_1 = \|H_F\psi_I\|$, let $\delta_2 = \|P_F\psi_I\|$, and let $\delta_3 = \|Q_F\psi_I\|$, where Q_F is a projection onto $Range\, H_F$. Also, let $g_F := E_2^f - E_1^f$.

Finally, we introduce the notion of what we will refer to as a generic Hamiltonian H_I.

Given an m–dimensional subspace V of $\mathbb{C}^N$, the natural question one can ask is what is a distance from the "typical" vector ψ_I to V. More specifically, suppose one has some reasonable probability distribution function for the vectors ψ_I on the unit sphere S^N in $\mathbb{C}^N$ (say uniform). Then the expected value of $\|\phi_I\|^2$ of the orthogonal projection ϕ_I of the ψ_I on V is equal to m/N. One can check that the probability of the event $\{\psi_I \in \mathbb{C}^N : |\|\phi_I\|^2 - m/N| \geq \alpha m/N\}$ is exponentially small in α (see *e.g.* [23]). Note now that $Q_F\psi_I$ is the projection of ψ_I onto the range of Q_F, which is an m–dimensional subspace. We therefore will call H_I *generic* if its ground state ψ_I satisfies $\|Q_F\psi_I\| = O(\sqrt{m/N})$.

Our first assertion is the non-existence result, showing that for any choice of H_I and any function $f(s)$ the running time cannot be smaller than τ_- defined below.

Theorem 3.1.1 (The lower bound on the running time)**.** *Consider the interpolating family Eq.* (3.1) *with an arbitrary f. Then the running time τ_- in Eq.* (3.2) *for which $\|P_F\psi_{\tau_-}(1)\| \geq 1/5$ satisfies*

$$\tau_- \;\geq\; \frac{1 - 5\|P_F\psi_I\|}{5\|H_F\psi_I\|}\,, \qquad \textit{for} \qquad \delta_2 < 1/5\,. \tag{3.3}$$

Remark 5.

1. This result shows that it is impossible to construct the family of the interpolating Hamiltonians $H(s)$ such that the evolution of Ψ_I will have a reasonable overlap with P_F if the running time τ is smaller than τ_-. To probe how tight this bound is, one wants to construct a specific family $H(s)$ and the running time τ_+ for which $\|P_F\psi_\tau(1)\|$ is not small, and make a comparison between $\tau_\pm$. One construction of such a $H(s)$ is presented in the next section. As we shall see, the bound τ_- is not tight ($\tau_-/\tau_+ - 1 \neq o(1)$), but of the right order of magnitude (meaning $\tau_-/\tau_+ = O(1)$) in terms of the asymptotic dependence on the small parameter m/N.

2. For a generic H_I both $\|H_F\psi_I\|$ and $\|P_F\psi_I\|$ are $O(\sqrt{m/N})$, hence the minimal running time τ cannot be smaller than $O(\sqrt{N/m})$.

3. As we will see, the (nearly) optimizing parametrization $f(s)$ is in fact non adiabatic.

Comparison with the Ioannou - Mosca result.

In [42], Ioannou and Mosca established the lower bound on the running time τ for a particular class of problems where the initial Hamiltonian H_I is diagonal in the Hadamard basis, while the problem Hamiltonian H_F is diagonal in the standard basis. Their result is non trivial provided the largest eigenspace of H_I has dimension $N - m$ where $m \ll \sqrt{N}$, and the lower bound they obtained is given by $\tau_- = O(\sqrt{N}/m)$. Since one can always interchange the roles of H_I and H_F and shift energy so that the largest eigenspace corresponds to the energy 0, their result can be viewed as a slightly weaker version of Theorem 3.1.1 for this class of Hamiltonians.

Proof. The proof is based on the following observation: Note that ψ_I is an approximate eigenvector of $H(s)$ since $(H(s) - (1 - f(s))E_I I)\psi_I = f(s)H_F\psi_I$, and the norm of the right hand side is equal to δ_1. So by the first order perturbation theory, the dynamical evolution of the state ψ_I given by (3.2) will stay close (up to the dynamical phase) to ψ_I, unless the running time τ is such that the total variation, given by $\tau\delta_1$, is of order 1. The proof below formalizes this argument.

For a solution $\psi_\tau(s)$ of (3.2), let

$$\phi_\tau(s) := \; e^{if_\tau(s)}\psi_\tau(s)\,, \quad f_\tau(s) = \tau\, E_I \int_0^s (1 - f(r))\,\mathrm{d}r\,. \tag{3.4}$$

Then one can readily check that $\phi_\tau(s)$ satisfies the IVP

$$i\dot{\phi}_\tau(s) \;=\; \tau\hat{H}(s)\phi_\tau(s)\,, \quad \phi_\tau(0) \;=\; \psi_I\,, \tag{3.5}$$

where

$$\hat{H}(s) \;=\; (1 - f(s))\,(H_I - E_I\, I) \;+\; f(s)\, H_F\,.$$

The factor $e^{if_\tau(s)}$ is usually referred to as a dynamical phase.

Let $U_\tau(t,s)$ be a semigroup generated by $\hat{H}(s)$, namely, $\phi_\tau(t) = U_\tau(t,s)\phi_\tau(s)$, $t \geq s$. Plug this in (3.5) we get $i\partial_s\, U_\tau^*(t,s)\phi_\tau(t) \;=\; \tau\hat{H}(s)U_\tau^*(t,s)\phi_\tau(t)$, and this implies

$$-i\,\partial_s\, U_\tau(t,s) \;=\; \tau\, U_\tau(t,s)\hat{H}(s)\,; \quad U_\tau(s,s) \;=\; I\,; \quad t \geq s\,. \tag{3.6}$$

Then the solution $\phi_\tau(1)$ of (3.5) is equal to $U_\tau(1,0)\,\psi_I$. On the other hand,

$$I \;-\; U_\tau(1,0) \;=\; \int_0^1 \partial_s\, U_\tau(1,s)\,\mathrm{d}s \;=\; i\,\tau \int_0^1 U_\tau(t,s)\hat{H}(s)\,\mathrm{d}s\,,$$

hence applying both sides on ψ_I we obtain

$$\psi_I \;-\; \phi_\tau(1) \;=\; i\,\tau \int_0^1 U_\tau(t,s)\hat{H}(s)\psi_I\,\mathrm{d}s\,.$$

We infer

$$\|\psi_I \;-\; \phi_\tau(1)\| \;\leq \tau \int_0^1 \|\hat{H}(s)\psi_I\|\,\mathrm{d}s\,.$$

But

$$\hat{H}(s)\psi_I \;=\; \{(1 - f(s))\,(H_I - E_I\, I) \;+\; f(s)\, H_F\}\,\psi_I \;=\; f(s)\, H_F\psi_I\,,$$

and we get the bound

$$\|\psi_I \;-\; \phi_\tau(1)\| \;\leq\; \tau\,\delta_1 \int_0^1 f(s)\,\mathrm{d}s \;\leq\; \tau\,\delta_1\,,$$

where in the last step we used $0 \leq f(s) \leq 1$. By the triangle inequality,

$$\begin{aligned} \Big| \|P_F\psi_I\| - \|P_F\phi_\tau(1)\| \Big| &\leq \|P_F\psi_I - P_F\phi_\tau(1)\| \leq \|\psi_I - \phi_\tau(1)\| \\ &\leq \tau\,\delta_1\,, \end{aligned}$$

so that

$$\|P_F\phi_\tau(1)\| \leq \tau\,\delta_1 + \delta_2\,.$$

On the other hand, by the assumption of the theorem $\|P_F\psi_\tau(1)\| \geq 1/5$, hence $\|P_F\phi_\tau(1)\| \geq 1/5$. As a result, we can bound

$$1/5 \leq \tau\,\delta_1 + \delta_2\,,$$

and the assertion follows. □

3.2 An explicit algorithm for solving general unstructured search

In this section, an explicit algorithm for solving general unstructured search is presented. It has two parts. The first part is the construction of a specific family $H(s)$ and the runtime τ_+ for which $\|P_F\psi_\tau(1)\| \geq 1/5$. The second part is a small counting subroutine where one actually determines the number of marked item.

The initial Hamiltonian chosen is $H_I = -|\psi_I\rangle\langle\psi_I|$, and we use a non adiabatic parametrization

$$f(s) = \begin{cases} 0\,, \text{ if } s = 0\,, \\ \alpha \equiv \frac{1}{1-E_F} \text{ if } s \in (0,1)\,, \\ 1 \text{ if } s = 1\,. \end{cases} \tag{3.7}$$

This means we move extremely quickly (instantly in fact) to the middle of the path, stay there for the time τ, and then move quickly again to the end of the path. With this choice of H_I and f, we have the following theorem on the running time.

Theorem 3.2.1 (The upper bound on the running time)**.** *With the choice of the rank one initial Hamiltonian $H_I = -|\psi_I\rangle\langle\psi_I|$ and f that satisfies Equ. 3.7, $\|P_F\psi_{\tau_+}(1)\| \geq 1/5$ for*

$$\tau_+ = \frac{C(1-E_F)}{|E_F|\,\|P_F\psi_I\|}\,, \tag{3.8}$$

and any value $C \in [1/3, 2/3]$, provided that $\|Q_F\psi_I\|/g_F = O(1/\ln N)$.

Remark 6.

1. For a generic choice of H_I, one has $\|Q_F\psi_I\| = O(\sqrt{m/N})$, $\|P_F\psi_I\| = O(\sqrt{m_1/N})$, where $m_1 = Rank\,P_F$. It implies that $\tau_-/\tau_+ = O(1)$ for $m = O(1)$.

2. This assertion can be viewed as an extension of the result obtained in [34] that considered the original Grover's search problem in the Hamiltonian–based algorithm.

3. The interpolating function f in this construction is similar to the one used in [34], namely, it is a double step function. Since f is discontinuous, we prefer to refer to this particular construction as the Hamiltonian–based algorithm rather than AQC.

There are two parameters, namely E_F and $\|P_F\psi_I\|$, that enter into τ_+ here. Note that a-priori both the values of E_F and $\|P_F\psi_I\|$ may be unknown. For instance, the value of the overlap $\|P_F\psi_I\|$ corresponds to the number of marked items which is *unknown* in the setup. A close look at the form of τ_+ reveals that τ_+ is not very sensitive to E_F, especially when E_F is very close to 0. On the other hand, τ_+ is very sensitive to the other parameter, $\|P_F\psi_I\|$. To this end, I present the following auxiliary result:

Theorem 3.2.2. *Suppose that the value of E_F is known. Then there is a Hamiltonian – based algorithm that determines $\|P_F\psi_I\|$ with $1/N^2$ accuracy and requires $O((\ln N)^2)$ of the running time.*

Remark 7.

1. The running time for this sub-algorithm is much shorter than τ_+, so it does not significantly affect the total running time.

2. A parallel result in the context of the quantum circuit model was establishes earlier in [15].

Proof of Theorem 3.2.1. First observe that regardless of the choice of $f(s)$ in (3.1) we have $\psi_\tau(s) \in Y$, where Y is a subspace of the Hilbert space, spanned by the vectors in the range of H_F and ψ_I. Here we have used the fact that the range of H_I by the assumption of the theorem coincides with $Span\{\psi_I\}$. Let us choose the orthonormal basis $\{e_i\}_{i=1}^{m+1}$ for Y as follows: The first m vectors in the basis are the eigenvectors of H_F corresponding to $\{E_i^f\}$ that differ from zero, and the last vector e_{m+1} is obtained from ψ_I using the Gram Schmidt procedure. That is,

$$e_{m+1} := \frac{\bar{Q}_F\psi_I}{\|\bar{Q}_F\psi_I\|} = \frac{\bar{Q}_F\psi_I}{\sqrt{1-\delta_3^2}}, \quad \bar{Q}_F = 1 - Q_F .$$

Our choice of g ensures that

$$\psi_\tau(1) = e^{-i\alpha\tau\cdot(E_F P_I + H_F)}\psi_I .$$

Here we introduce P_F as the orthogonal projection onto the span of $\{e_i\}$ with $E_i^f = E_1^f$, and P_{m+1} the orthogonal projection onto e_{m+1}. Clearly

$$P_{m+1} = \frac{\bar{Q}_F\, P_I\, \bar{Q}_F}{1-\delta_3^2}$$

We want to compute the matrix elements of the propagator $e^{-i\alpha\tau(H_I+H_F)}$ in the basis $\{e_i\}$. To this end, we observe that in this basis $H_F = diag(E_F, \ldots, E_m^f, 0)$, and H_I is a block matrix such that

$$\left\| E_F P_I \,-\, \left[\begin{array}{cc} 0 & \delta_3 V^* \\ \delta_3 V & E_F \end{array}\right] \right\| \;\leq\; 3\delta_3^2 |E_F|\,, \tag{3.9}$$

where $\|V\| = |E_F|$. Indeed, we have

$$\begin{aligned} \|Q_F\; P_I\; Q_F\| \;&=\; \delta_3^2\,, \\ \|P_{m+1}\; P_I\; P_{m+1}\| \;&=\; 1-\delta_3^2\,, \\ \|P_{m+1}\; P_I\; Q_F\| \;&=\; \delta_3\,(1-\delta_3^2)^{1/2}\,. \end{aligned}$$

To get the last equality, notice since P_I is rank 1, $\left\|\bar{Q}_F P_I \bar{Q}_F P_I Q_F\right\| = (1-\delta_3^2)\left\|\bar{Q}_F P_I Q_F\right\|$. On one hand, $\left\|\bar{Q}_F P_I Q_F\right\| \leq \left\|\bar{Q}_F P_I\right\| \|P_I Q_F\| = \delta_3(1-\delta_3^2)^{1/2}$. On the other hand, $\left\|\bar{Q}_F P_I Q_F x\right\| = \left\|\bar{Q}_F P_I \frac{P_I Q_F x}{\|\bar{Q}_F P_I x\|}\left\|\bar{Q}_F P_I x\right\|\right\| = (1-\delta_3^2)^{1/2}\|P_I Q_F x\|$ for any $x \in \mathbb{R}^{m+1}$.

Together, we obtain that in this basis

$$\left\| E_F P_I \,+\, H_F \,-\, \left[\begin{array}{cc} D & \delta_3 V^* \\ \delta_3 V & E_F \end{array}\right] \right\| \;\leq\; 3\delta_3^2 |E_F|\,,$$

where $D = diag(E_F, \ldots, E_m^f)$. A simple perturbative argument (*cf.* Duhamel formula (3.11) below) shows that

$$\left\| e^{-i\alpha\tau\cdot(E_F P_I + H_F)} \,-\, e^{-i\alpha\tau K} \right\| \;\leq \left\| e^{i\alpha\tau K} e^{-i\alpha\tau\cdot(E_F P_I + H_F)} - I \right\| \leq\; 3\delta_3^2 |E_F| \alpha\tau\,, \tag{3.10}$$

with

$$K \;=\; \left[\begin{array}{cc} D & \delta_3 V^* \\ \delta_3 V & E_F \end{array}\right].$$

To this end, we split K into the diagonal and off diagonal parts:

$$K \;=\; K_1 \,+\, K_2 := \left[\begin{array}{cc} D & 0 \\ 0 & E_F \end{array}\right] + \left[\begin{array}{cc} 0 & \delta_3 V^* \\ \delta_3 V & 0 \end{array}\right].$$

Let

$$\Omega(s) := \; e^{i\alpha\tau s K_1}\, e^{-i\alpha\tau s K}\,; \quad K_2(s) := \; e^{i\alpha\tau s K_1}\, K_2\, e^{-i\alpha\tau s K_1}\,,$$

then $\dot{\Omega}(s) = -i\alpha\tau K_2(s)\Omega(s)$, and $e^{-i\alpha\tau K}$ is given by the following Duhamel formula:

$$\begin{aligned} e^{-i\alpha\tau K} \;&=\; e^{-i\alpha\tau K_1}\left\{ I \,-\, i\alpha\tau \int_0^1 K_2(s)\Omega(s)\,\mathrm{d}s \right\} && (3.11) \\ &=\; e^{-i\alpha\tau K_1}\left\{ I \,-\, i\alpha\tau \int_0^1 K_2(s)\,\mathrm{d}s \right. \\ &\qquad \left. +\; (-i\alpha\tau)^2 \int_0^1 K_2(s)\,\mathrm{d}s \int_0^s K_2(r)\Omega(r)\,\mathrm{d}r \right\}. && (3.12) \end{aligned}$$

Observe now that

$$[K_2(s)]_{1,m+1} \;=\; [K_2]_{1,m+1}\;,$$

since $e^{-i\frac{\tau}{2}sK_1}$ is diagonal with $(1,1)$ entry equal to $(m+1,m+1)$ entry. In fact, $[K_2(s)]_{j,m+1} = [K_2]_{j,m+1}$ for all j such that $E_j^f = E_1^f$. Therefore

$$\left\| P_F \int_0^1 K_2(s)\,\mathrm{d}s\, P_{m+1} \right\| \;=\; \delta_2\,|E_F|\,, \tag{3.13}$$

since

$$P_F\,K_2\,P_{m+1} \;=\; \frac{|E_F|}{\sqrt{1-\delta_3^2}}\,P_F\,P_I\,P_{m+1}\,.$$

To estimate the second term in (3.12), we note first that the following bound holds:

Lemma 3.2.3. *We have*

$$\left\| \int_0^s P_{m+1}\,K_2(r)\,Q_F\,\bar{P}_F\,\Omega(r)\,\mathrm{d}r \right\| \;\le\; \frac{8\delta_3}{\tau g_F} \;+\; \frac{2\delta_3^2}{g_F}\,. \tag{3.14}$$

This estimate is essentially a content of Lemma 3.3 in [**?**]. The idea is that, since the spectral supports of K_1 for P_{m+1} and $Q_F\bar{P}_F$ are a distance g_F apart, the integral over r has a highly oscillating phase of order τg_F. For completeness, we prove this lemma below.

Armed with this estimate and using the fact that $K_2(s)$ is off diagonal, we get

$$\begin{aligned}
&\left\| P_F \int_0^1 K_2(s)\,\mathrm{d}s \int_0^s K_2(r)\Omega(r)\,\mathrm{d}r\, P_{m+1} \right\| \\
&=\; \|P_F\,K_2\,P_{m+1}\| \cdot \left\| P_{m+1} \int_0^1 \mathrm{d}s \int_0^s K_2(r)\Omega(r)\,\mathrm{d}r\, P_{m+1} \right\| \\
&\le\; |E_F|\,\delta_2 \,\cdot \int_0^1 \mathrm{d}s \left\| \int_0^s P_{m+1}K_2(r)(P_F + Q_F\bar{P}_F)\Omega(r)P_{m+1}\mathrm{d}r \right\| \\
&\le\; |E_F|\,\delta_2 \,\cdot \left\{ \int_0^1 \|P_{m+1}\,K_2(r)\,P_F\|\;\mathrm{d}r \right. \\
&\left. +\; \max_{s\in[0,1]} \left\| \int_0^s P_{m+1}\,K_2(r)\,Q_F\,\bar{P}_F\,\Omega(r)\,\mathrm{d}r \right\| \right\}\,,
\end{aligned}$$

where we have used $\|\Omega(r)\| = \|P_{m+1}\| = 1$ and (3.13). Applying estimates (3.13) and (3.14), we bound

$$\begin{aligned}
&\left\| P_F \int_0^1 K_2(s)\,\mathrm{d}s \int_0^s K_2(r)\Omega(r)\,\mathrm{d}r\; P_{m+1} \right\| \\
&\qquad\le\; |E_F|\,\delta_2 \,\cdot \left\{ |E_F|\,\delta_2 \;+\; \frac{8\delta_3}{\tau g_F} \;+\; \frac{2\delta_3^2}{g_F} \right\}\,.
\end{aligned} \tag{3.15}$$

Multiplying (3.12) by P_F from the left and by P_{m+1} from the right, and using the estimates (3.13) and (3.15), we establish

$$\begin{aligned}\left\|P_F\, e^{-i\alpha\tau K}\, P_{m+1}\right\| \;&\geq\; \alpha\tau \left\|P_F \int_0^1 K_2(s)\,\mathrm{d}s\, P_{m+1}\right\| \\ &- (\alpha\tau)^2 \left\|P_F \int_0^1 K_2(s)\,\mathrm{d}s \int_0^s K_2(r)\Omega(r)\,\mathrm{d}r\, P_{m+1}\right\| \\ &=\; \alpha\tau|E_F|\,\delta_2\cdot\left(1 \,-\, \alpha\tau\,\cdot\left\{|E_F|\delta_2 \,+\, \frac{8\delta_3}{\tau g_F} \,+\, \frac{2\delta_3^2}{g_F}\right\}\right). \qquad (3.16)\end{aligned}$$

Now

$$\begin{aligned}\|P_F\psi_F(1)\| \;&=\; \left\|P_F e^{-i\alpha\tau\cdot(E_F P_I + H_F)}\psi_I\right\| \\ &=\; \|P_F e^{-i\alpha\tau\cdot(E_F P_I + H_F)} Q_F\psi_I \\ &\quad + P_F(e^{-i\alpha\tau\cdot(E_F P_I + H_F)} - e^{-i\alpha\tau\cdot K})P_{m+1}\psi_I + P_F e^{-i\alpha\tau\cdot K} P_{m+1}\psi_I\| \\ &\geq\; \left\|P_F e^{-i\alpha\tau\cdot K} P_{m+1}\right\| - 3\delta_3^2\|E_F\|\alpha\tau - \delta_3\,.\end{aligned}$$

So combining the estimates in (3.10), and (3.16), the result will follow provided

$$\begin{aligned}&\alpha\tau|E_F|\,\delta_2\cdot\left(1 \,-\, \alpha\tau\,\cdot\left\{|E_F|\delta_2 \,+\, \frac{8\delta_3}{\tau g_F} \,+\, \frac{2\delta_3^2}{g_F}\right\}\right) \\ &\qquad\geq\; 1/5 \,+\, \delta_3 \,+\, 3\delta_3^2|E_F|\alpha\tau\,.\end{aligned}$$

Note now that for $\tau = O(1/\delta_2)$ the above inequality is satisfied for values of τ and δ_3 such that

$$\alpha\tau|E_F|\,\delta_2\cdot(1 \,-\, \alpha\tau|E_F|\delta_2\,) \;\geq\; 2/9\,, \quad \delta_3/g_F = O(1/\ln N)\,.$$

The result now follows. □

Proof of Lemma 3.2.3. Let

$$X := \frac{1}{2\pi i}\oint_\Gamma P_{m+1}\,(K_1 - zI)^{-1}\,K_2\,(K_1 - zI)^{-1}\,Q_F\,\bar{P}_F\,\mathrm{d}\,z\,, \qquad (3.17)$$

where the contour Γ is a circle $\{z\in\mathbb{C}:\ |z - E_F| = g_F/2\}$. Since

$$\frac{1}{2\pi i}\oint_\Gamma (K_1 - zI)^{-1}\,\mathrm{d}\,z \;=\; P_F \,+\, P_{m+1}\,,$$

one can readily check that

$$[X\,,\,K_1] \;=\; P_{m+1}\;K_2\,Q_F\,\bar{P}_F\,.$$

Hence

$$\begin{aligned}&\int_0^s P_{m+1}\,K_2(r)\,Q_F\,\bar{P}_F\,\Omega(r)\,\mathrm{d}r \\ &\qquad=\; \frac{-2i}{\tau}\int_0^s \frac{d}{\mathrm{d}r}\Big(e^{-i\frac{\tau}{2}rK_1}\,X\,e^{i\frac{\tau}{2}rK_1}\Big)\,\Omega(r)\,\mathrm{d}r\,.\end{aligned}$$

Integrating the right hand side by parts, we obtain

$$\begin{aligned}
&\int_0^s P_{m+1}\, K_2(r)\, Q_F\, \bar{P}_F\, \Omega(r)\, \mathrm{d}r \\
&= -\frac{2i}{\tau}\left\{ e^{-i\frac{\tau}{2}rK_1}\, X\, e^{i\frac{\tau}{2}rK_1}\, \Omega(r)\Big|_0^s - \int_0^s e^{-i\frac{\tau}{2}sK_1}\, X\, e^{i\frac{\tau}{2}sK_1}\, \dot{\Omega}(r)\, \mathrm{d}r \right\} \\
&= -\frac{2i}{\tau}\, e^{-i\frac{\tau}{2}rK_1}\, X\, e^{i\frac{\tau}{2}rK_1}\, \Omega(r)\Big|_0^s - \int_0^s e^{-i\frac{\tau}{2}sK_1}\, X\, e^{i\frac{\tau}{2}sK_1}\, K_2(r)\Omega(r)\, \mathrm{d}r\,.
\end{aligned}$$

The first term is bounded in norm by $4\frac{\|X\|}{\tau}$, while the second one is bounded by $\|X\| \cdot \|K_2\|$. It follows from (3.17) that $\|X\| \leq \frac{2\|K_2\|}{g_F}$. On the other hand, $\|K_2\| = \delta_3\|V\| = |E_F|\delta_3 \leq \delta_3$ by (3.9), and the result follows. □

Proof of Theorem 3.2.2. The algorithm used in the proof is inspired by the mean ergodic theorem and makes use of the fact that the survival probability $c_F(t) = \langle\psi_I|e^{itH_F}|\psi_I\rangle$ is directly measurable in AQC framework. We suggest to measure the survival probability for a number a times specified below to estimate the overlap δ_2, and then to count the total running time spent on this subroutine.

Our starting point is a truncated Taylor's expansion for e^x:

$$e^x \;=\; \sum_{k=0}^{L} \frac{x^k}{k!} \;+\; O\!\left(\frac{|x|^L}{L!}\right).$$

Setting $x = pe^{iw}$, and multiplying both sides by x^{-p}, we obtain the following relation:

$$e^{p(\cos w - 1)} e^{ip\sin w} \;=\; e^{-p} \sum_{k=0}^{L} \frac{p^k e^{iwk}}{k!} \;+\; O\!\left(e^{-p}\frac{p^L}{L!}\right). \tag{3.18}$$

If $1 - \cos w > g$, then the left hand side of Eq. (3.18) is bounded by e^{-pg} and therefore is smaller than $1/N^2$, provided $p = 2\ln N/\min(1, g)$. On the other hand, with such choice of p, the remainder term in Eq. (3.18) is bounded by $O(1/N^2)$ if L is chosen to be equal to ep. Combining these observations, we get

$$e^{-p}\sum_{k=0}^{ep} \frac{p^k e^{ik\omega}}{k!} \;=\; \begin{cases} 1 + O(1/N^2)\,, & \text{if } \omega = 0 \\ O(1/N^2)\,, & \text{if } 1 - \cos\omega > g \end{cases}, \tag{3.19}$$

where $p = 2\ln N/\min(g, 1)$.

Now, using the spectral decomposition of H_F,

$$e^{it(H_F - E_F)} = \sum_{i=1}^{N} P_i e^{it(E_i^f - E_F)} P_i,$$

where E_i is the i-th distinct eigenvalue of H_F and P_i is the projector onto the spectral subspace associated with E_i. Hence

$$e^{-p}\sum_{t=0}^{ep}\frac{p^k}{k!}\,\langle\psi_I|e^{it(H_F-E_F)}\psi_I\rangle \;=\; (\delta_2)^2+O(1/N^2)\,, \tag{3.20}$$

for $p=2\ln N/\min(1,1-\cos g_F)$ where we have used Eq. (3.19). The total running time is $\sum_{t=1}^{ep} t = O((\ln N)^2)$. □

3.3 Robust adiabatic quantum computing

In this section, I present a necessary technical requirement on the quantum device for AQC Grover's search to be successful. The $\sqrt{N}$ speedup in AQC algorithm obtained in the tractable problems (*c.f.* [22] for the Grover's problem or its rigorous treatment in [43]) relies on a special choice of the parametrization $f(s)$ in (3.1). Namely, it is constructed in such a way that $\dot{f}(s)$ is small at instances $\{s_j\}$ at which the spectral gap $g(s_j) := \lambda_2(s_j)-\lambda_1(s_j)$ of $H(s_j)$ is small. In the AQC jargon, it is usually referred to as the quantum search by local adiabatic evolution. It is interesting to compare this approach with the construction used in Theorem 3.2.1, where this strategy is pushed to the extreme, namely, f used there is actually constant except for the endpoints $s=0,1$ where it jumps. There are two practical problems with this approach:

1. The values $\{s_j\}$ obviously depend on H_F and in particular on E_F (even for the Grover's problem, as the simple scaling argument shows). So to choose such an f, one has to know the spectral structure of H_F with $o(1/\sqrt{N})$ precision. This is tacitly assumed in [22].

2. Even if this technical obstacle can be overcome, the extreme susceptibility of $\psi_\tau(1)$ to the parametrization f poses a radical problem in practical implementation. Indeed, it is presumably extremely difficult to enforce $\dot{f}=0$ for a long stretch of the physical time, as the realistic computing device inevitably fluctuates due to the presence of the noise. Some models that try to take into the account the noise were proposed, see *e.g.* [20, 6], but to the best of our knowledge, all of the existing constructions contain ad hoc parameters and are not derived from the first principles. For some interesting rigorous work in this direction that considers de-phasing open systems see [9].

Another issue that will motivate this result is related to the fact that the adiabatic theorems fall into two categories: Those that describe the solutions for *all* times, including times $s\in[0,1]$, and those that characterize the solutions at large times $s>1$, where the Hamiltonian is time independent again. Interestingly, they give more precision for long times. We call

the first category, the one that applies to all times, uniform, the second is the long time category.

A representative result from the uniform category is the following, see *e.g.*, [8]:

Theorem 3.3.1 (Uniform adiabatic theorem)**.** *Suppose that the $H(s)$ is twice differentiable and bounded family of self adjoint operators on the interval $[0,1]$ that is τ–independent, and suppose in addition that*

$$g \;:=\; \mathrm{dist}(\lambda_1(s), \sigma(H(s) \setminus \lambda_1(s)) \;>\; 0 \quad \textit{for all } s \in [0,1]\,. \tag{3.21}$$

Then the solution $\psi_\tau(s)$ of the IVP (3.2) *satisfies*

$$\lim_{\tau\to\infty} \mathrm{dist}\,(\psi_\tau(s), \textit{Range } P_F) \;=\; 0\,. \tag{3.22}$$

A characteristic result (see, *e.g.* [12, 59, 57]) which lies in the long time category is

Theorem 3.3.2 (Long time adiabatic theorem)**.** *Suppose that the $H(s)$ is smooth (that is C^∞ class) and bounded family of self adjoint operators with $\dot{H}(s)$ supported on $[0,1]$ that is τ–independent, and suppose in addition that* (3.21) *holds as well. Then the solution $\psi_\tau(s)$ of the IVP* (3.2) *satisfies*

$$\mathrm{dist}\,(\psi_\tau(s), \textit{Range } P_F) \;=\; o(\tau^{-n}) \textit{ for } s \geq 1\,, \tag{3.23}$$

for any $n \in \mathbb{N}$.

Remark 8.

1. In words, one can say that starting and finishing the interpolation slowly decreases the error in the adiabatic theorem.

2. There is, in general, no uniformity in n; the term on the right hand side is of order $c_n\tau^{-n}$, where c_n grows rapidly with n (*c.f.* the following discussion).

3. The distinction between the uniform and the long time AT has an analog in integrals. Suppose that $g(s) \in C^\infty([0,1])$. Then

$$\int_0^s g(t)e^{it\tau}dt \;=\; \begin{cases} o(\tau^{-n})\,, \text{ if } s \geq 1\,; \\ O(\tau^{-1}) \text{ if } s \in (0,1)\,. \end{cases}$$

In the application to AQC it is natural to investigate the dependence of the coefficients c_n in terms of the gap g and minimize the running time τ in such a way that $c_n\tau^{-n} = o(1)$ for some optimally chosen value n. The recent result in this direction, [54], gives $\tau = O(g^{-3})$. For the sketch of the argument that uses (truncated) Nenciu's expansion technique [29] and how it leads to the sharper estimate $\tau = O(g^{-2}|\ln g|^5)$, see [26]. One is then tempted to

combine the starting and finishing slowly strategy with the quantum search by local adiabatic evolution strategy in order to minimize the error in the adiabatic theorem. Such analysis was undertaken recently for Grover's search problem in [61].

Inspired by the above discussion, we will assume that in the robust setting for any given moment s inside the interval J described below, (and which excludes the vicinities of the endpoints $s = 0, 1$) the value $\dot{f}(s)$ is greater than some small but fixed $\kappa > 0$. To motivate the definition of J, suppose that the function f lies in the long time category, *i.e.,* $\dot{f}$ is supported in $[0, 1]$ and f is smooth. Let $b \in [0, 1]$ be such that $\ddot{f}$ does not change sign on $[b, 1]$ (but it can vanish there). It is not difficult to see that since f is monotone, f has to be concave on $[b, 1]$; hence $\ddot{f} \leq 0$ there. Now let us define the interval J for *any* differentiable function f. Let $a = \min_{s\in[0,1]}\{f(s) = 1/3\}$. Let $b = \min_{s\in[0,1]}\{f(s)$ is concave on $[s, 1]\}$. We then define the interval $J := [a, b]$ for $f \in C^1$ provided $a \leq b$, $J = \emptyset$ if $a > b$, and $J := [a, 1]$ if $f \notin C^1$. To illustrate this notion, consider $f \in \mathbb{C}^\infty(\mathbb{R})$ constructed as follows:

$$f(t) \;=\; \int_{-\infty}^{t} g(s)ds\,, \quad g(s) \;=\; \begin{cases} 0\,, \text{ if } s \notin [0, 1]\,; \\ \alpha\, e^{\frac{1}{s(s-1)}} \text{ if } s \in (0, 1)\,. \end{cases}$$

The factor α here is a normalization constant, chosen so that $f(1) = 1$. We then have

$$\ddot{f}(t) \;=\; \left(\frac{1}{t^2} \,-\, \frac{1}{(1-t)^2}\right) g(t)\,, \text{ for } t \in [0, 1]\,,$$

so that the only inflection point is $t = 1/2$. Hence f is convex on $[0, 1/2]$ and is concave on $[1/2, 1]$. We therefore get $b = 1/2$ and $J = [f^{-1}(1/3), 1/2]$. The convexity of f on $[0, 1/2]$ implies that $f(y) - f(x) \geq \dot{f}(x)(y - x)$ for any $x, y \in [0, 1/2]$. Choosing $x = s$, $y = 0$, we obtain $\dot{f}(s) \geq f(s)/s$ for $s \in (0, 1/2]$. Since f is monotone, we conclude that $\dot{f}(s) \geq 2/3$ on $[a, 1/2]$. So, in this example $\kappa = 2/3$.

The utility of the introduction of the interval J is as follows: On the interval $[a, 1]$ the function f is concave, hence it satisfies $f(y) - f(x) \leq \dot{f}(x)(y - x)$ for any $x, y \in [b, 1]$. In particular, we have

$$1 - f(t) \;\leq\; \dot{f}(t)(1 - t) \;\leq\; \dot{f}(t) \text{ for } t \in [b, 1]\,, \tag{3.24}$$

the relation we are going to exploit.

The following result establishes that in the case of the small rank initial Hamiltonian the robust version of AQC does not yield a significant speedup unless κ can be made exponentially small:

Theorem 3.3.3 (Robust lower bound on the running time)**.** *Suppose that f in Eq.* (3.1) *is (piecewise) differentiable and satisfies $\dot{f}(s) \geq \kappa > 0$ for $s \in J$ with the interval J defined above. Also, let us assume that $E_I = -1$. Then, if $\tau < \tau_r = O\left(\frac{\kappa}{m^2\delta^2 \ln \delta}\right)$, we have*

$$|\langle\psi_I|\psi_\tau(1)\rangle| \;>\; \frac{4}{5} \,+\, 2\delta\,, \tag{3.25}$$

where $\delta = \|Q_I Q_F\|$. *Hence the running time* τ *for which* $\|Q_F \psi_\tau(1)\| \geq 1/5$ *cannot be smaller than* τ_r.

Remark 9.

1. This theorem tells us that for a generic H_I of the small rank, the robust running time τ_r cannot be smaller than $O(\kappa N/\ln N)$. Hence, unless the control precision κ is on the order of $O(\ln N/\sqrt{N})$, AQC is not much better than its classical counterpart that solves GUS for $\tau = O(N)$.

2. As we remarked earlier, the requirement $E_I = -1$ is a very mild one.

Proof of Theorem 3.3.3. First, the following inequality shows when $|\langle\psi_I|\psi_\tau(1)\rangle| > 4/5 + 2\delta$, $\|Q_F\psi_\tau(1)\| < 1/5$.

$$\begin{aligned}
1 &= \|Q_F\psi_\tau(1)\|^2 + \|(1-Q_F)\psi_\tau(1)\|^2 \\
&\geq \|Q_F\psi_\tau(1)\|^2 + \|Q_I(1-Q_F)\psi_\tau(1)\|^2 \\
&= \|Q_F\psi_\tau(1)\|^2 + \langle\psi_\tau(1)(Q_I - Q_FQ_I - Q_IQ_F + Q_FQ_IQ_F)\psi_\tau(1)\rangle \\
&\geq \|Q_F\psi_\tau(1)\|^2 + \|Q_I\psi_\tau(1)\|^2 - 2\delta \\
&\geq \|Q_F\psi_\tau(1)\|^2 + |\langle\psi_I|\psi_\tau(1)\rangle|^2 - 2\delta
\end{aligned}$$

Now, let us remind the reader that in the context of this assertion $E_I = -1$. As in the proof of theorem 3.1.1,

$$\phi_\tau(s) := e^{if_\tau(s)}\psi_\tau(s)\,, \quad f_\tau(s) = -\tau\int_0^s (1-f(r))\,\mathrm{d}r\,.$$

and

$$\hat{H}(s) = (1-f(s))\,(H_I+1) + f(s)\,H_F\,.$$

Let us introduce the auxiliary matrix

$$B(s) = (f(s)H_F + 1 - f(s) + \epsilon i))^{-1}\,,$$

and let $\phi(s) = \psi_I - f(s)H_FB(s)\,\psi_I$, where ϵ is a small parameter to be chosen later. Omitting the s dependence, we have

$$\hat{H}\phi = -f(1-f)H_IH_FB\,\psi_I - i\epsilon f H_F B\,\psi_I\,. \tag{3.26}$$

That means that away from the m values of s for which $B^{-1}(s)$ has zero eigenvalue, $\|\hat{H}\phi\|$ is very small, since $\|H_IH_F\psi_I\| \leq \delta^2$. Note now that by fundamental theorem of calculus we have

$$\langle\phi(1)|\phi_\tau(1)\rangle = \langle\phi(0)|\phi_\tau(0)\rangle + \int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\,ds\,, \tag{3.27}$$

where $\phi_\tau(s)$ is defined in (3.4). But $\langle\phi(0)|\phi_\tau(0)\rangle = 1$ and

$$\begin{aligned} |\langle\phi(1)|\phi_\tau(1)\rangle| &= \left|\langle\psi_I|\phi_\tau(1)\rangle - \langle\psi_I|\frac{H_F}{H_F - \epsilon\, i}|\phi_\tau(1)\rangle\right| \\ &\leq |\langle\psi_I|\phi_\tau(1)\rangle| + \|Q_F\psi_I\| = |\langle\psi_I|\phi_\tau(1)\rangle| + \delta\,. \end{aligned}$$

Substitution into Eq. (3.27) gives

$$1 - |\langle\psi_I|\phi_\tau(1)\rangle| \leq \left|\int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\, ds\right| + \delta\,.$$

Hence Eq. (3.25) will follow if

$$\left|\int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\, ds\right| < \frac{1}{5} - 3\delta\,. \tag{3.28}$$

To establish the above bound, we note first that

$$\frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle = \langle\dot\phi(s)|\phi_\tau(s)\rangle - i\tau\langle\phi(s)|\hat H(s)|\phi_\tau(s)\rangle\,. \tag{3.29}$$

We bound the first term on the right hand side by $\|\dot\phi\|$ and the second one by $\tau\|\hat H\phi\|$. On the other hand, suppressing the s-dependence, we have

$$\dot\phi = -\dot f H_F B\psi_I - f\dot f B(H_F - 1)BH_F\psi_I\,,$$

hence

$$\|\dot\phi\| \leq \dot f\,\|B\|\,\|H_F\psi_I\| + 2\dot f\,\|B\|^2\,\|H_F\psi_I\|\,,$$

where we have used $|f| \leq 1$ and $\dot f \geq 0$. Let $\mathrm{dist}(S, z)$ be an Euclidean distance from the set S to the point z in $\mathbb{C}$, and let $\sigma(H)$ stand for the spectrum of H. Then we can estimate the right hand side further as

$$\|\dot\phi\| \leq \frac{\dot f\delta}{\Delta_\epsilon} + \frac{2\dot f\delta}{(\Delta_\epsilon)^2}\,, \tag{3.30}$$

with

$$\Delta_\epsilon(s) := \mathrm{dist}(f(s)\sigma(H_F)\,,\, -1 + f(s) + \epsilon\, i)$$

and where we have used $-Q_F \leq H_F \leq Q_F$. Taking the norm from the both sides of (3.26) we get that

$$\|\hat H\phi\| \leq \|H_IQ_F\|\,\|fH_FB\|\,\|Q_F\psi_I\| + \epsilon\,\|fH_FB\|\,\|Q_F\psi_I\|\,, \tag{3.31}$$

where we have used $H_FQ_F = H_F$ and $\|H_IQ_F\| \leq \|Q_IQ_F\|$, with the later relation following from

$$\|H_IQ_F\| = \|H_IQ_IQ_F\| \leq \|H_I\|\,\|Q_IQ_F\|\,.$$

To estimate $\|fH_FB\|$ we consider three cases:

1. $s \in [0, a]$: On this interval we can estimate

$$\|f(s)H_F B(s)\| \;\leq\; \max_{s\in[0,a]} \frac{1}{\Delta_\epsilon(s)} \;\leq\; 3\,, \tag{3.32}$$

   where we have used $\sigma(H_F) \subset [-1, 1]$.

2. $s \in J$: In this case, we bound

$$\|f(s)H_F B(s)\| \;\leq\; \frac{1}{\Delta_\epsilon(s)} \;\leq\; \frac{\dot{f}(s)}{\kappa\Delta_\epsilon(s)} \tag{3.33}$$

   using theorem's hypothesis.

3. $s \in [b, 1]$: Here we estimate

$$\begin{aligned}\|f(s)H_F B(s)\| \;&=\; \left\|f(s)H_F\left(f(s)H_F + 1 - f(s) + \epsilon i)\right)^{-1}\right\| \\ &\leq\; 1 + \frac{(1-f(s)) + \epsilon}{\Delta_\epsilon(s)} \;\leq\; 2 + \frac{\dot{f}(s)}{\Delta_\epsilon(s)}\end{aligned} \tag{3.34}$$

   where in the last step we have used (3.24).

Plugging (3.32) – (3.34) into (3.31), we obtain

$$\|\hat{H}\phi\| \;\leq\; (\delta^2 + \epsilon\delta)\left(3 + \frac{\dot{f}(s)}{\kappa\Delta_\epsilon}\right). \tag{3.35}$$

Using (3.30) and (3.35) to bound the right hand side of (3.29), we get

$$\left|\frac{d}{ds}\langle\phi|\phi_\tau\rangle\right| \;\leq\; \frac{\dot{f}\delta}{\Delta_\epsilon} + \frac{2\dot{f}\delta}{(\Delta_\epsilon)^2} + \tau(\delta^2 + \epsilon\delta)\left(3 + \frac{\dot{f}(s)}{\kappa\Delta_\epsilon}\right). \tag{3.36}$$

In what follows we will use

Lemma 3.3.4. *We have bounds*

$$\int_0^1 \frac{\dot{f}ds}{\Delta_\epsilon} \;\leq\; -2(m+1)\ln\epsilon\,; \quad \int_0^1 \frac{\dot{f}ds}{(\Delta_\epsilon)^2} \;\leq\; \frac{2(m+1)}{\epsilon}\,. \tag{3.37}$$

Integrating both sides of (3.29) over s and using (3.36) and (3.37), we arrive at

$$\left|\int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\, ds\right| \;\leq\; 3\tau(\delta^2 + \epsilon\delta) + 2(m+1)\delta\left(-\ln\epsilon\left(1 + \frac{\tau\delta}{\kappa} + \frac{\tau\epsilon}{\kappa}\right) + \frac{2}{\epsilon}\right).$$

Hence the required bound in Eq. (3.28) follows with the choice $\epsilon = 10^3(m+1)\delta$, provided $\tau \leq -\frac{C\kappa}{\epsilon^2\ln\epsilon}$ where C is some generic constant. □

Proof of Lemma 3.3.4. We derive the first bound, the second bound can be shown analogously. To this end, we observe that

$$\begin{aligned}\frac{\dot{f}}{\Delta_\epsilon} &= \max_{E_n\in\sigma(H_F)} \frac{\dot{f}}{|fE_n+1-f-\epsilon\, i|} \\ &< \sum_{E_n\in\sigma(H_F)} \frac{\dot{f}}{|f(E_n-1)+1-\epsilon\, i|}\end{aligned}$$

It follows that

$$\begin{aligned}\int_0^1 \frac{\dot{f}ds}{\Delta_\epsilon} &< \sum_{E_n\in\sigma(H_F)} \int_0^1 \frac{\dot{f}ds}{|fE_n+1-f-\epsilon\, i|} \\ &\leq (m+1) \max_{E\in[-1,1]} \int_0^1 \frac{\dot{f}ds}{|fE+1-f-\epsilon\, i|}\,,\end{aligned}$$

where $m = Rank\ H_F$. But

$$\begin{aligned}&\int_0^1 \frac{df}{\sqrt{(f(E-1)+1)^2+\epsilon^2}} \\ &\quad= \frac{1}{E-1}\ln\left((E-1)f+1+\sqrt{((E-1)f+1)^2+\epsilon^2}\right)\Big|_0^1 \\ &\quad= \frac{1}{E-1}\ln\left(\frac{E+\sqrt{E^2+\epsilon^2}}{1+\sqrt{1+\epsilon^2}}\right).\end{aligned}$$

One can check by taking the derivative that the expression on the right hand side is monotonically decreasing for all $E\in[-1,1]$. Since it is also positive and continuous, this term achieves its maximum at $E=-1$, with the value

$$-\frac{1}{2}\ln\left(\frac{\sqrt{1+\epsilon^2}-1}{1+\sqrt{1+\epsilon^2}}\right) \leq -2\ln\epsilon$$

for ϵ small enough. Hence the first bound in (3.37) follows. □

3.4 Gaps in the spectrum of the interpolating Hamiltonian

Although the size of the gap in the spectrum of $H(s)$ did not play any role in the proofs, it is instructive to estimate it for two reasons. The first is that the size of the gap manifests

itself in the adiabatic theorem of quantum mechanics (see Theorem 3.3.1), on which AQC is built. The second is that physicists believe the existence of such a gap makes AQC more robust then QCM, as it protects the ground state against excitement which is the cause of decoherence. To AQC to be meaningful, one should choose the initial Hamiltonian H_I in such a way that *Rank* P_I is small. The error in the adiabatic evolution (the right hand side of (3.22)) depends on the size of the gap g, with the rough upper bound on the error of the form $\frac{C}{\tau g^3}$ [43].

Theorem 3.4.1 (The size of the gap)**.** *Let $g_I := E_2^i - E_I$ be a gap between the ground state of the initial Hamiltonian H_I and the rest of its spectrum, where the rank of H_I is assumed to be small. Let $\delta_4 := \|P_I Q_F\|$, where Q_F is a projection onto the range of H_F. Then we have the following estimate on the size of the gap g in* (3.21)*:*

$$g \;\leq\; 10\,\delta_4\,, \tag{3.38}$$

provided $g_I > 3\delta_4$.

Remark 10. In fact, one can relax the condition $g_I > 3\delta_4$, but to keep the presentation simple we impose this additional constraint.

Proof of Theorem 3.4.1. The main tool we are going to use is the so called Krein's formula for the rank m perturbation of the initial Hamiltonian H_I. It gives a characterization of the location of m eigenvalues of the perturbed matrix that *differ* from the spectral values of H_I. Specifically, let A, B be two hermitian matrices, with *Rank* $B = m$, and let Q be an orthogonal projection onto *Range* B. Suppose that A is invertible (that is $0 \notin \sigma(A)$), let's consider when $A + tB$ contains eigenvalue 0. $A + tB$ can be decomposed as $\bar{Q}A\bar{Q} \bigoplus \big(tBQ + QAQ - QA\bar{Q}(\bar{Q}A\bar{Q})^{-1}\bar{Q}AQ\big)$. From Schur complement formula, which says that if A is invertible then

$$QA^{-1}Q \;=\; \big(QAQ \;-\; QA\bar{Q}\,(\bar{Q}A\bar{Q})^{-1}\,\bar{Q}AQ\big)^{-1}\,,$$

where $\bar{Q} := I - Q$ and the inverses on the right hand side are understood as acting on the ranges of $\bar{Q}$ and Q, respectively, $A + tB$ is similar to $\bar{Q}A\bar{Q} \bigoplus (tBQ + K^{-1})$, with

$$K := QA^{-1}Q\,.$$

So 0 is an eigenvalue of $A + tB$ if and only if the $m \times m$ matrix $K^{-1} + tBQ$ contains 0 in its spectrum. $K^{-1} + tBQ$ is interpreted as acting in the m–dimensional space *Range* B. To apply the Krein's formula in our context, we form a one parameter family

$$H_t := \; H_I + tH_F\,, \quad t = \frac{s}{1-s}\,, \quad t \in [0,\infty)\,.$$

It then follows that for a fixed $t \in (0,\infty)$ the eigenvalues of H_t that differ from $\sigma(H_I)$ are given by the roots of the equation

$$\det\big(K^{-1}(E) \;+\; tH_F Q_F\big) \;=\; 0\,, \tag{3.39}$$

where

$$K(E) := Q_F \, (H_I \, - \, E)^{-1} \, Q_F \, .$$

Whenever it is clear from the context that we are working with the operators on *Range* Q_F, we will suppress the Q_F dependence.

To analyze (3.39), we start with the following simple observation:

Lemma 3.4.2. *The matrix $K(E)$ can be decomposed as*

$$K(E) \; = \; \hat{K}(E) \, + \, \frac{\delta_4^2 \, D}{E_I - E} \, . \tag{3.40}$$

Here the matrix D is positive semi-definite, and is bounded in norm by 1. The matrix $\hat{K}(E)$ is holomorphic in the half plane Re $E > E_I - g_I/2$ and is positive definite for $E \in [E_I - g_I/2, E_I + g_I/2]$. Moreover, in this interval we have bounds

$$\frac{2}{4+g_I} - \delta_4^2 \; \leq \; \hat{K}(E) \; \leq \; \frac{2}{g_I} \, ; \quad \frac{4}{(4+g_I)^2} - \delta_4^2 \; \leq \; \frac{d\hat{K}(E)}{dE} \; \leq \; \frac{4}{g_I^2} \, . \tag{3.41}$$

In applications to the AQC the parameter δ_4 is typically extremely small: $\delta_4^2 = O(1/N)$. Hence the second contribution in (3.40) is small provided $|E - E_I| \gg \delta_4$. Therefore for value of E in such intervals, we can first find the roots $\hat{E}_i(t)$ of

$$\det \left(\hat{K}^{-1}(E) \, + \, t H_F \right) \; = \; 0 \, , \tag{3.42}$$

and then estimate $|\hat{E}_i(t) - E_i(t)|$, where $E_i(t)$ are corresponding roots of (3.39). As we will see, the level crossings or the avoided level crossings for H_t occur for values of t such that a pair of eigenvalues $E_k(t)$, $E_l(t)$ is close to E_I. To find these values of t in the first approximation, we fix the value $E = E_I$ in (3.42) and solve it for t. We have

Lemma 3.4.3. *The equation*

$$\det \left(\hat{K}^{-1}(E_I) \, + \, t H_F \right) \; = \; 0 \, , \tag{3.43}$$

has exactly m_+ roots $\{t_j\}_{j=1}^{m_+}$ on $(0, \infty)$, where m_+ is a number of negative eigenvalues of H_F.

We are now in position to estimate the size of the gap g from above. Namely, we consider the gaps g_j for H_t for $t = t_j$. Since $t = \frac{s}{1-s}$ and $H(s) = (1-s)H_t$, we obtain $g \leq \frac{g_j}{1+t_j} \leq g_j$. Let

$$\beta := \; 2 \left(\frac{\delta_4^2}{\frac{4}{(4+g_I)^2} - \delta_4^2} \right)^{1/2} \, .$$

To get a bound on g_j we show that (3.39) has roots in the intervals $[E_I - \beta, E_I)$ and $(E_I, E_I + \beta]$, at $t = t_j$. We then infer that $g_j \leq 2\beta$, from which the upper bound in (3.38) follows

since $\beta < 5\delta_4$. Observe first that by condition of the Theorem 3.4.1, $\sigma(H_I) \cap [E_I - \beta, E_I) = \sigma(H_I) \cap (E_I, E_I + \beta] = \emptyset$ (where the latter property follows from the bound $\beta > 4\delta_4 > g_I$), hence we are in position to use Lemma 3.4.2. We only show that for the first interval, the proof is analogous for the second one.

To this end, we will denote by $\mathrm{sgn}(A)$ the signature of the matrix A. We observe that since $\frac{\delta_4^2 D}{E_I - E}$ in (3.40) is positive semidefinite and monotone increasing for the values of E in $[E_I - \beta, E_I)$, we have

$$\mathrm{sgn}(K^{-1}(E_I - 0) + t_j H_F) \;\leq\; \mathrm{sgn}(\hat{K}^{-1}(E_I) + t_j H_F)\,. \tag{3.44}$$

On the other hand, we have

$$\hat{K}(E_I) - \hat{K}(E_I - \beta) \;=\; \int_{E_I - \beta}^{E_I} \hat{K}'(E)\,\mathrm{d}E \;\geq\; \beta \left(\frac{4}{(4 + g_I)^2} - \delta_4^2 \right), \tag{3.45}$$

where in the last step we have used (3.41). Hence

$$\begin{aligned} K(E_I - \beta) &= \hat{K}(E_I - \beta) + \frac{\delta_4^2 D}{\beta} \\ &\leq \hat{K}(E_I) - \left(\beta \left(\frac{4}{(4 + g_I)^2} - \delta_4^2 \right) I - \frac{\delta_4^2 D}{\beta} \right) \\ &\leq \hat{K}(E_I) - \frac{\delta_4^2}{\beta} I < \hat{K}(E_I)\,, \end{aligned} \tag{3.46}$$

with a choice of β as above, and where we have used $\|D\| \leq 1$. We infer

$$K^{-1}(E_I - \beta) + t_j H_F \;>\; \hat{K}^{-1}(E_I) + t_j H_F\,,$$

and since the matrix $\hat{K}^{-1}(E_I) + t_j H_F$ has zero eigenvalue by construction, we obtain

$$\mathrm{sgn}(K^{-1}(E_I - \beta) + t_j H_F) \;<\; \mathrm{sgn}(\hat{K}^{-1}(E_I) + t_j H_F)\,. \tag{3.47}$$

Combining (3.44) and (3.47) together, we get

$$\mathrm{sgn}(K^{-1}(E_I - \beta) + t_j H_F) \;<\; \mathrm{sgn}(K^{-1}(E_I + 0) + t_j H_F)\,. \tag{3.48}$$

But the family $K^{-1}(E) + t_j H_F$ is continuous on $[E_I - \beta, E_I)$, hence there should be some value of E in this interval for which $K^{-1}(E) + t_j H_F$ has the eigenvalue 0. □

Proof of lemma 3.40. We decompose

$$\begin{aligned} K(E) &= Q_F\,(H_I - E)^{-1}\,Q_F \\ &= Q_F \bar{P}_I\,(H_I - E)^{-1}\,Q_F + Q_F P_I\,(H_I - E)^{-1}\,Q_F\,. \end{aligned}$$

The first contribution will correspond to $\hat{K}(E)$ in (3.40), and the second one to its counterpart in (3.40). Note now that for $E \in [E_I - g_I/2, E_I + g_I/2]$ we have

$$\frac{g_I}{2}\,\bar{P}_I \;\leq\; \bar{P}_I(H_I - E) \;\leq\; \left(2 + \frac{g_I}{2}\right)\,\bar{P}_I\,,$$

where the the upper bound is a consequence of $\|H_I\| = 1$. Hence we obtain

$$\frac{2}{4+g_I}\,Q_F\bar{P}_IQ_F \;\leq\; Q_F\bar{P}_I(H_I - E)^{-1}Q_F \;\leq\; \frac{2}{g_I}\,Q_F\bar{P}_IQ_F\,.$$

Therefore, the first bound in (3.41) follow now from

$$Q_F\bar{P}_IQ_F \;=\; Q_F \,-\, Q_FP_IQ_F$$

and

$$0 \;\leq\; Q_FP_IQ_F \;\leq\; \delta_4^2\,Q_F\,.$$

To obtain the second bound in (3.41) we note that

$$\frac{d}{dE}\,(H_I \,-\, E)^{-1} \;=\; (H_I \,-\, E)^{-2}$$

for $E \notin \sigma(H_I)$, and then proceed as above. □

Proof of lemma 3.4.3. Let $A := \hat{K}(E_I)$, then it follows from previous lemma that $0 < A$. Hence

$$\left(A^{-1} \,+\, tH_F\right) \;=\; tA^{-1/2}\left(t^{-1} \,+\, A^{1/2}H_FA^{1/2}\right)A^{-1/2}\,.$$

The right hand side is not invertible for values $\{t_j\}$ such that

$$-t_j^{-1} \;\in\; \sigma\left(A^{1/2}H_FA^{1/2}\right)\,,$$

and the result follows now from Sylvester's law of inertia [41]. □

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