

**NON-DERIVATION OF  
THE QUANTUM BOLTZMANN EQUATION  
FROM THE PERIODIC VON NEUMANN EQUATION**

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**Abstract**

We consider the quantum dynamics of an electron in a periodic box of large size  $L$ , for long time scales  $T$ , in  $d$  dimensions of space,  $d \geq 3$ . One obstacle occupying a volume 1 is present in the box. The coupling constant between the electron and the obstacle is  $\lambda$ . The model is described by a scaled periodic Von Neumann equation with a potential, a time-reversible equation. We investigate the asymptotic dynamics in the typical low-density regime  $T \sim L^d$ ,  $L \rightarrow \infty$ . The coupling constant has to be rescaled and small, namely  $\lambda \sim L^{-d+2} \rightarrow 0$ . More general regimes are in fact considered. Our analysis is easily adapted in the case of Dirichlet boundary conditions.

Loosely speaking, the dynamics of an electron moving in a field of obstacles and in the low-density regime is, “in general”, asymptotically described by a time-irreversible Boltzmann equation. Large finite boxes are often used in the physical literature to formally justify this statement. However, the above asymptotics has only been proved true for “randomly” distributed obstacle, say. On the more, the physical derivations relying on taking large finite boxes are mathematically as well as physically questionable.

Starting from these observations, we investigate here in a quantitative way the case of an electron moving on a large periodic (or Dirichlet) box, with a given deterministic obstacle. We prove here that both periodicity and the fact that the obstacle is deterministic, create strong phase coherence effects which dominate the asymptotic process. This implies that, (a) the limiting dynamics is not the Boltzmann equation, (b) it is time-reversible, (c) it is the same for any time scale  $T$  such that, roughly,  $T/L^2 \rightarrow \infty$ , and (d) the unusual rescaling of  $\lambda$  is needed as well. However, the convergence proved here only holds as a term-by-term convergence of certain series.

Our result relies on the analysis of certain Riemann sums with arithmetic constraints, and number theoretic considerations relating the asymptotic distribution of integer vectors on spheres of large radius happen to play a key rôle in this paper.

**Key words:** Quantum Boltzmann equation, low-density limit, reversibility, irreversibility, sums of squares, Waring’s problem.

**AMS subject classification:** 76P05, 11P05, 35Q40, 35B10, 81U05.

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# 1 Introduction

In this paper we are interested in the quantum dynamics of an electron in a periodic distribution of obstacles in  $d$  dimensions of space ( $d \geq 3$ ). To be precise, the electron is assumed to evolve on a periodic box (a torus), so that our analysis relies on Fourier series rather than on Bloch waves. Note however that our analysis is easily adapted in the case of Dirichlet boundary conditions. We do not give the easy details on this point.

The size of the period is measured by the large scaling parameter  $L$ , and each elementary cell contains one obstacle occupying a volume of the order  $O(1)$ . Also the coupling constant measuring the strength of the interaction between the electron and the obstacle is denoted by  $\lambda$ . We consider the asymptotic dynamics as  $L \rightarrow \infty$ . In order to obtain a non-trivial limiting dynamics, one has to rescale time as well, and to look at the evolution of the electron on long time scales of the order  $T$ , with  $T \rightarrow \infty$ . The present paper is essentially concerned with the regime  $T/L^2 \rightarrow \infty$ : we need a time scale which is long enough to “see” the finite size of the box. Also, our analysis is naturally restricted to the unusual case of a small coupling  $\lambda \sim L^2/T \rightarrow 0$ . We refer to (2.6) and (2.7) for the precise regime. For dimensions  $d \geq 3$ , the time scales under consideration here include the standard low-density scaling (or Boltzmann-Grad scaling), where the ratio  $T \sim L^d$  is prescribed. The latter scaling is important since in this case the obstacles occupy a proportion  $\sim 1/L^d$  of the total volume, so that the probability for the electron to hit an obstacle once per unit time on this time scale is unity.

The present system is a particular case of the more general problem of describing the large time dynamics of an electron in a field of obstacles. Such a system is described by a scaled, linear von Neumann equation. In the general case, i.e. when the distribution of obstacles is arbitrary enough, and if the coupling with the obstacles is sufficiently small, it is physically expected (see e.g. [VH1], [VH2], [VH3], [KL1], [KL2], [Ku], [Pr], [Vk], [Zw] or also [Cal], see [Fi] for recent developments) that the system actually tends to be described by a Boltzmann equation in the limit. One usually identifies two main regimes: in the low density regime, the electron hits an obstacle once per unit time in the macroscopic time scale and each interaction is of the order unity ; in the weak coupling regime, the electron hits an obstacle  $1/\varepsilon$  times per unit time in the macroscopic time scale and each interaction is of the order  $\varepsilon$ , for some small  $\varepsilon \rightarrow 0$ . Such situations are routinely considered in the modeling of semi-conductor devices, and the use of the Boltzmann equation in place of the underlying long time Schrödinger or von Neumann equation is standard, see for example [MRS]. The motivation of the present work is based on two observations.

First, many physical derivations of the Boltzmann equation starting from the von Neumann equation are based on the use of large finite boxes. In particular, our approach tries to mimic the elementary derivation of Fermi’s Golden Rule based on time-dependent scattering theory which can be found in many textbooks e.g. [Boh], [CTDRG], [CTDL], [Mes], [SSL], and which has been recently revived in [Co]. This is where our limit in  $L$  originates. We recall that Fermi’s Golden Rule gives the expression of the transition rate involved in the limiting Boltzmann equation for

the electron. Elementary time-dependent scattering theory [Boh] considers indeed a Hamiltonian of the form  $H_0 + V$  in a finite box of size  $L$ , where  $H_0$  is the free kinetic energy. Initially, particles are supposed concentrated on an eigenstate  $\psi_n$  of  $H_0$  associated with the energy  $\varepsilon_n \approx n^2/L^2$ . The goal is to compute the time asymptotics of the population  $|C_p(t)|^2 = |(\psi(t), \psi_p)|^2$  of the initially void states of energy  $\varepsilon_p$ ,  $p \neq n$ , where  $\psi(t)$  denotes the wave-function of the particle at time  $t$ . It is well known that, if the energy levels remain discrete (i.e. if the size of the box is left unchanged), the behaviour of  $|C_p(t)|^2$  is either an oscillatory function of time if the energies are different ( $\varepsilon_p \neq \varepsilon_n$ ) or a quadratic function of time if the energies are equal ( $\varepsilon_p = \varepsilon_n$ ), but can by no means be a linear function of time. However, scattering theory aims at producing a rate of change of the populations, i.e. a probability per unit of time. Therefore, one looks for a linear in time behaviour of  $|C_p(t)|^2$ . To remove this apparent paradox, one must therefore let the size of the box go to infinity. Indeed, when the level spacings are set to zero, i.e. as  $L \rightarrow \infty$ , the oscillatory function of time  $|C_{\mathbf{p}}(t)|^2$ , where now  $\mathbf{p}$  is a continuous variable ranging in the wave-vector space  $\mathbb{R}^3$ , formally is, in the sense of distributions in the  $\mathbf{p}$  variable, asymptotic as time goes to infinity to a linear function of time multiplied by a delta function of the differences of the energies of the initial and final states  $\delta(\varepsilon_{\mathbf{n}} - \varepsilon_{\mathbf{p}})$ . In this sense, one recovers the usual Fermi Golden Rule as a succession of two limits  $L \rightarrow \infty$  then  $t \rightarrow \infty$ . In particular, the process of taking the size of the box to infinity is of primary importance and not just a technicality, because one cannot deal from the onset with an infinite medium: in an infinite box, the eigenstates of the unperturbed Hamiltonian  $H_0$  are not normalized, and therefore unphysical, and it cannot be given any meaning to the quantity  $|C_p(t)|^2$ . Needless to say, the procedure of taking at the same time the above two limits is mathematically questionable, and the physical relevance of this approach is also discussed and questioned in detail in [Co]. Similar difficulties are encountered in other formal derivations (see e.g. [Cal]), where the dynamics of an electron in a large finite box is considered, and the underlying low-density or weak coupling limit, together with the limit of an infinitely large box, are formally taken simultaneously, a doubtful procedure.

Secondly, many rigorous mathematical works establish precise convergence results of the von Neumann equation towards a Boltzmann equation in various situations where the obstacles are, say, randomly distributed (see e.g. [Sp], [HLW], [La], [EY]). In particular, the initially time-reversible model is proved to be asymptotically described by a time-irreversible equation, but the convergence holds in expectation value (roughly). Hence the result typically fails for some “zero-measure set” of configurations of the obstacles. This is due to the fact that the limiting equation is time-irreversible. However, these works do not give any quantitative information about the specific configurations of obstacles where the convergence actually fails.

Starting from these two observations, the present paper deals at variance with a model which is deterministic. On the more, the problem is set in a given, periodic (or Dirichlet) box at once. This is a very strong constraint as well as a non-generic case. Our goal is to test at a quantitative level what happens in this

very particular configuration. We wish to exhibit an effective setting where the formal convergence towards a Boltzmann equation actually fails. Note that the deterministic and periodic situation has been previously studied in [Ca2] (see also [CD]), but a small damping parameter  $\alpha > 0$  is introduced in this paper, which models the interaction of the electron with external light ([NM], [SSL]), and technically, it acts as a regularizing parameter. In [Ca2], the low-density asymptotics followed by the limit  $\alpha \rightarrow 0$  gives the desired convergence towards a Boltzmann equation. In this picture, the present paper performs the two limits in the reversed order (limit in  $\alpha$  and then low density limit) and our results show that the two limits do not commute.

Roughly summarizing, the results presented here are twofold. On the one hand, we show in this paper that the present model *is not* described by a Boltzmann equation in the limit, and the actual limiting dynamics is proved to be *time-reversible* (Theorem 1). On the more, the limiting dynamics is the same for any time scale  $T$  such that, roughly,  $T/L^2 \rightarrow \infty$ , and not only in the low-density case where  $T \sim L^d$  is prescribed. However, we emphasize that we only prove here the convergence towards the limiting dynamics in the sense of a *term-by-term* convergence of certain series. On the other hand, the non-convergence result in Theorem 1 turns out to be related to the presence of phase coherence effects, quantified in Theorem 2, and which are specific to the case of an electron in a box with periodic or Dirichlet boundary conditions. Number theoretic considerations happen to have great importance in describing the limiting dynamics. In particular, Theorem 1 relies on the explicit computation of the limit of certain Riemann sums with quadratic constraints of the type,  $\lim_{L \rightarrow \infty} \frac{1}{L^{2d-2}} \sum_{(n,p) \in \mathbb{Z}^{2d}} \phi\left(\frac{n}{L}, \frac{p}{L}\right) \mathbf{1}[n^2 = p^2]$ ,

where  $\phi$  is any smooth and decaying function (Theorem 2). This second result is of independent interest and relies on a precise number theoretical analysis performed in [CP]. Note that when the dimension  $d = 3$ , the above mentioned convergence relies on a conjecture of number theoretical nature (see assumption **(A)**). Note also that the emergence of number theoretical considerations in the context of the periodic Schrödinger equation is fairly natural and actually standard, see e.g. [Bo1], [Bo2].

We end this introduction with one important comment. The present paper exhibits one particular, deterministic geometry, where the natural infinite volume and low-density limits do not lead to any Boltzmann equation, contrary to what is expected in more general geometries or distributions of obstacles. We may stress however that the present non convergence result is somehow not surprising, at least at an intuitive level, due to the specificity of the periodic case. In particular, we wish to mention that a similar (though not strictly equivalent) situation holds in the context of classical mechanics : the dynamics of a classical particle in a stochastic distribution of obstacles is known to be asymptotically described by a linear Boltzmann equation in the appropriate low-density limit [BBS]; however, when the obstacles are periodically distributed, such a result is known to be false [BGW]. The non-convergence result proved in [BGW] relies on number theoretical

considerations specific to the periodic context as well.

A review about the non-convergence result presented here and the convergence result proved in [Ca2], can be found in [Ca4].

## 2 Presentation of the results

### 2.1 The mathematical model under consideration

Mathematically speaking, the situation presented in the introduction is described by the following von Neumann equation on the torus  $(\mathbb{R}/2\pi L\mathbb{Z})^d$ ,

$$\frac{i}{T} \frac{\partial}{\partial t} \tilde{\rho}(t, \mathbf{x}, \mathbf{y}) = -\Delta_{\mathbf{x}} \tilde{\rho} + \Delta_{\mathbf{y}} \tilde{\rho} + \lambda(V(\mathbf{x}) - V(\mathbf{y})) \tilde{\rho}. \quad (2.1)$$

In this equation the unknown is the so-called density-matrix of the electron,  $\tilde{\rho}(t, \mathbf{x}, \mathbf{y})$ , which is the mathematical object describing the state of the electron at time  $t \in \mathbb{R}$  (see [CTDL]). It depends on a time variable  $t$  and two space variables  $\mathbf{x}$  and  $\mathbf{y}$  both belonging to the torus of period  $L$ ,  $(\mathbb{R}/2\pi L\mathbb{Z})^d$ . The interaction with the obstacle is taken into account through the potential  $\lambda V(\mathbf{x}) \in \mathbb{R}$ , where  $V(\mathbf{x})$  is the potential created by the obstacle in the elementary cell of size  $L$ , and  $\lambda \in \mathbb{R}$  is a coupling constant which scales the strength of the interaction. Throughout this paper the potential is assumed to be fixed (independently of  $L$ ), smooth, and compactly supported in the open elementary cell  $]0, 2\pi L[^d$ . Note that time scales of the order  $T$  are indeed considered in (2.1), due to the prefactor  $1/T$  in front of the time derivative  $\partial/\partial t$ .

Now the asymptotic process  $T \rightarrow \infty$  together with  $L \rightarrow \infty$  in (2.1) is performed in the Fourier space rather than directly on (2.1). For this reason, we need to define, for any  $n$  and  $p \in \mathbb{Z}^d$ , the following Fourier transforms,

$$\rho(t, n, p) := \int_{[0, 2\pi L]^{2d}} \tilde{\rho}(t, \mathbf{x}, \mathbf{y}) \frac{1}{(2\pi L)^{\frac{d}{2}}} \exp\left(-i \frac{n \cdot \mathbf{x}}{L}\right) \frac{1}{(2\pi L)^{\frac{d}{2}}} \exp\left(+i \frac{p \cdot \mathbf{y}}{L}\right) d\mathbf{x} d\mathbf{y}, \quad (2.2)$$

as well as the more standard,

$$\widehat{V}(\mathbf{n}) := \int_{[0, 2\pi L]^d} V(\mathbf{x}) \exp(-i\mathbf{n} \cdot \mathbf{x}) d\mathbf{x} \quad \left( = \int_{\mathbb{R}^d} V(\mathbf{x}) \exp(-i\mathbf{n} \cdot \mathbf{x}) d\mathbf{x} \right), \quad (2.3)$$

for any  $\mathbf{n} \in \mathbb{R}^d$ . The last equality comes from the assumption on the support of  $V$ , and  $\widehat{V}(\cdot)$  is by assumption a fixed profile belonging to the Schwartz-class  $\mathcal{S}(\mathbb{R}^d)$ . Here, bold letters  $\mathbf{n}, \mathbf{p}, \dots$  denote continuous variables belonging typically to  $\mathbb{R}^d$ , whereas plain letters  $n, p, \dots$  denote discrete variables belonging typically to  $\mathbb{Z}^d$ , a convention used throughout the paper. With these notations, the original von

Neumann equation (2.1) becomes,

$$\begin{aligned} \frac{i}{T} \frac{\partial}{\partial t} \rho(t, n, p) &= \frac{n^2 - p^2}{L^2} \rho(t, n, p) \\ &+ \frac{\lambda}{L^d} \sum_{k \in \mathbb{Z}^d} \left\{ \widehat{V} \left( \frac{n-k}{L} \right) \rho(t, k, p) - \widehat{V} \left( \frac{k-p}{L} \right) \rho(t, n, k) \right\}. \end{aligned} \quad (2.4)$$

Note that the transformation (2.2) is the natural one since the functions  $\psi_n(\mathbf{x}) := (2\pi L)^{-d/2} \exp(-in \cdot \mathbf{x}/L)$ , when  $n \in \mathbb{Z}^d$ , are the eigenfunctions of the operator  $-\Delta_{\mathbf{x}}$  on the space of periodic functions in the box  $[0, 2\pi L]^d$ , with degenerate eigenvalues,  $E_n := n^2/L^2$  ( $n \in \mathbb{Z}^d$ ). Note in particular that the limiting procedure  $L \rightarrow \infty$  performed in the present paper makes the spectrum of the Laplacian  $-\Delta_{\mathbf{x}}$  continuous.

Now, as it is standard in this field (see e.g. [Ku], [KL1], [KL2], [Cal], [Zw]) we are only interested in performing the asymptotics  $L \rightarrow \infty$ ,  $T \rightarrow \infty$  in (2.8) for particular initial data which are stationary states of the free von Neumann equation  $iT^{-1} \partial \tilde{\rho} / \partial t = (-\Delta_{\mathbf{x}} + \Delta_{\mathbf{y}}) \tilde{\rho}$ . In other words, we wish to quantify the large time influence of the potential for initial states which are equilibrium states of the unperturbed hamiltonian  $-\Delta_{\mathbf{x}}$ . The initial data of interest in the present paper are thus taken of the form,

$$\rho(t, n, p) \Big|_{t=0} = \frac{1}{L^d} \rho^0 \left( \frac{n}{L} \right) \mathbf{1}[n = p], \quad (2.5)$$

where  $\rho^0(\mathbf{n}) \geq 0$  ( $\mathbf{n} \in \mathbb{R}^d$ ) is assumed to be some given profile belonging to the Schwartz-class  $\mathcal{S}(\mathbb{R}^d)$ , and  $\mathbf{1}[n = p]$  denotes the indicator function of the set  $\{n = p\}$ . It is easily seen that the assumption (2.5) generalizes both the case of initial thermodynamical equilibrium where  $\rho(t, n, p) \Big|_{t=0} \approx L^{-d} \exp(-\beta n^2/L^2) \mathbf{1}[n = p]$ , and  $\beta$  is the inverse temperature, and the more general case where  $\rho(t = 0)$  is an arbitrary function of the energy  $\rho(t, n, p) \Big|_{t=0} \approx L^{-d} f(n^2/L^2) \mathbf{1}[n = p]$  for some ‘‘reasonable’’ function  $f$ .

There remains to quantify the exact regime under which  $L$  and  $T$  go to infinity in the present study. As mentioned before, one natural asymptotics in the present context is dictated by the low-density-regime where  $T \sim L^d$  and the coupling constant  $\lambda$  is of the order  $O(1)$ . It turns out that the present periodic situation dictates a slightly different and in some sense more general scaling. Indeed, let us rename the scaling parameters  $\lambda$  and  $T$ , and define the new scaling variables,

$$\mathcal{T} = TL^{-2}, \quad \Lambda = \lambda T. \quad (2.6)$$

With this renaming, the low-density scaling reads  $\mathcal{T} \sim L^{d-2}$ ,  $\Lambda \sim \mathcal{T}$ . Now, the asymptotics treated in this paper reads,

$$\begin{cases} \mathcal{T} \rightarrow \infty, \quad L \rightarrow \infty, \quad \Lambda = O(1), \quad \text{with } \frac{\mathcal{T}}{L^{\delta(d)} \log L} \rightarrow \infty, \\ \text{and } \delta(d) = 0 \text{ when } d \geq 5, \\ \delta(d) > 0 \text{ may be arbitrarily small when } d = 3, \text{ or } d = 4. \end{cases} \quad (2.7)$$

It describes a long time and small coupling regime, and (2.7) turns out to be the natural scaling in the present periodic situation.

We now wish to give some important comments and justifications for the scaling (2.7). Firstly, the condition  $\mathcal{T}/(L^{\delta(d)} \log L) \rightarrow \infty$  includes the important low-density-limit  $\mathcal{T} \sim L^{d-2}$  for dimensions  $d \geq 3$  as a particular case, and the reader may safely restrict his attention to the mere low-density regime throughout this paper. The very condition  $\mathcal{T}/(L^{\delta(d)} \log L) \rightarrow \infty$  stems from technical reasons, and the logarithmic factor originates both from the periodicity and from the fact that  $\sum_{j=1}^L 1/j \sim \log L$  as it will be clear later. We refer, for instance, to Section 3 on this point. Essentially, the conditions on  $\mathcal{T}$  mean that we are on a long enough time scale so as to “see” the geometry of the box. Recall indeed that the typical spacing between energy levels in the present case precisely is  $1/L^2$ . Secondly, the small coupling condition  $\Lambda = O(1)$  is much more restrictive than the condition  $\Lambda \sim \mathcal{T}$  imposed in the standard low-density scaling. However, this condition turns out to be again the natural one in the present periodic situation, see e.g. Theorem 1. Hence one readily observes on (2.7) two specificities of the periodic situation in comparison with the case of an electron in a “generic” distribution of obstacles: firstly, the time scale for which a satisfactory limiting dynamics is obtained can be either smaller or arbitrarily larger than the usual low-density time-scale (cases  $\mathcal{T} \sim L^\varepsilon$  for some small  $\varepsilon > 0$ , and  $\mathcal{T} \sim L^N$  for some large  $N$  respectively), and the limiting dynamics turns out to be the same in any case as we shall see (Theorem 1). This readily contrasts with the “generic” situation where fairly different limiting dynamics are expected depending on the time-scales under consideration. Secondly, the periodic situation imposes to rescale the strength of the potential with the time-scale as  $\Lambda \sim 1$ , in contrast with the low-density scaling where the correct values are  $\Lambda \sim \mathcal{T}$  when  $T \sim L^{d-2}$ . The rough mathematical reason for this second phenomenon is the following. On the time scale given in (2.7), and in particular on the low-density time-scale, the von Neumann equation reads  $i\partial_t \rho = \mathcal{T}[n^2 - p^2]\rho + \dots$ . For this reason, the resonances occurring when  $n^2 = p^2$  are emphasized as soon as  $\mathcal{T} \rightarrow \infty$  (e.g. due to the Riemann-Lebesgue Lemma, see Lemma 1 below). It turns out that the contribution of these resonances in the sum  $(1/L^{d-2}) \sum_{k \in \mathbb{Z}^d} \dots$  in (2.8) below is  $O(1)$ . This explains the need for a rescaling. In the random situation, we rather have  $i\partial_t \rho(t, \mathbf{n}, \mathbf{p}) = \mathcal{T}[\mathbf{n}^2 - \mathbf{p}^2]\rho + \dots$  where  $\mathbf{n}$  and  $\mathbf{p}$  are now continuous variables (roughly speaking), and much more subtle oscillation phenomena dominate (e.g. the non-stationnary phase Lemma), hence the fairly different behaviour in this case.

As a conclusion of this presentation, we may summarize from (2.6) and (2.4) that the present paper treats the asymptotics (2.7) on the equation,

$$\begin{aligned} \frac{\partial}{\partial t} \rho(t, n, p) &= -i\mathcal{T}[n^2 - p^2]\rho(t, n, p) \\ &- i \frac{\Lambda}{L^{d-2}} \sum_{k \in \mathbb{Z}^d} \left\{ \widehat{V} \left( \frac{n-k}{L} \right) \rho(t, k, p) - \widehat{V} \left( \frac{k-p}{L} \right) \rho(t, n, k) \right\}, \end{aligned} \quad (2.8)$$

for initial data of the form (2.5). Note that for notational convenience, the dependence of the solution  $\rho$  to (2.8) upon the parameters  $\mathcal{T}$ ,  $L$  and  $\Lambda$  is not made

explicit, a convention kept throughout this paper. We thus write  $\rho$  instead of  $\rho^{\mathcal{T},L,\Lambda}$  and allow ourselves to write  $\lim_{\mathcal{T} \rightarrow \infty} \rho$  and so on.

## 2.2 Comparison with other works: “badly sampled” oscillatory sums

Let us introduce now the distribution  $f(t, \mathbf{n}) := \sum_{n \in \mathbb{Z}^d} \rho(t, n, n) \delta(\mathbf{n} - \frac{n}{L})$  as a distribution on  $\mathbb{R}^d$ , where  $\rho$  satisfies (2.8). We mentioned in the introduction that, at least in the general case of an electron in an arbitrary distribution of obstacles, the underlying von Neumann equation is physically expected to converge towards a Boltzmann equation in the low-density limit. In the specific case under consideration here, the above rough statement means (should it hold true) that the distribution  $f(t, \mathbf{n})$  should converge in the low-density regime towards some  $f^\infty(t, \mathbf{n})$  satisfying the so-called Quantum Boltzmann equation,

$$\partial_t f^\infty(t, \mathbf{n}) = 2\pi \int_{\mathbb{R}^d} \delta(\mathbf{n}^2 - \mathbf{k}^2) [\sigma(\mathbf{n}, \mathbf{k}) f^\infty(t, \mathbf{k}) - \sigma(\mathbf{k}, \mathbf{n}) f^\infty(t, \mathbf{n})] d\mathbf{k}, \quad (2.9)$$

for some function  $\sigma(\mathbf{n}, \mathbf{k})$  representing the transition rate between the impulse  $\mathbf{n}$  and the impulse  $\mathbf{k}$ . Here,  $\sigma$  is given by a series in  $\lambda$  (the so-called Born-series), whose first term is,

$$\sigma(\mathbf{n}, \mathbf{k}) = \lambda^2 |\widehat{V}(\mathbf{n} - \mathbf{k})|^2 + O(\lambda^3), \quad (2.10)$$

and this last equation is called the Fermi Golden Rule (See [RS]). From a mathematical point of view, results of this type have actually been proved true in [Sp], [HLW], [La], [EY], when the potential  $\lambda V$  is chosen to be stochastic, i.e.  $\lambda V \equiv \lambda V(x, \omega)$ ,  $\omega$  belonging to some probability space, and the convergence holds *in expectation* with respect to  $\omega$  (to be more precise, the weak coupling limit leads to (2.9) with a cross-section given by the first term of the expansion (2.10), whereas the low-density regime leads to (2.9) with the full Born-series expansion (2.10)). In the deterministic situation where the potential is given at once, we wish to quote the work of F. Nier [Ni1], [Ni2] for the derivation of the scattering rate  $\sigma$  mentioned above. All these mathematical works deal with an electron evolving in the whole space at once (and not in a finite box). Let us also mention [Ca1] for a non-convergence result when the period  $L$  is fixed of the order  $O(1)$ . Finally, we wish to quote that the equation (2.8) *modified* by a damping parameter  $\alpha > 0$  is considered in [Ca2] (see also [CD]),

$$\begin{aligned} \frac{i}{T} \frac{\partial}{\partial t} \rho(t, n, p) &= \frac{n^2 - p^2}{L^2} \rho(t, n, p) - i\alpha \rho(t, n, p) \mathbf{1}[n \neq p] \\ &+ \frac{\lambda}{L^d} \sum_{k \in \mathbb{Z}^d} \left\{ \widehat{V}\left(\frac{n-k}{L}\right) \rho(t, k, p) - \widehat{V}\left(\frac{k-p}{L}\right) \rho(t, n, k) \right\}, \end{aligned} \quad (2.11)$$

(compare with (2.4)), and the initial datum is assumed of the form (2.5) as well. In [Ca2], the low-density limit is performed first and the asymptotics  $\alpha \rightarrow 0$  is taken in a second step: the resulting limiting dynamics is then proved to be (2.9)



with the correct cross-section  $\sigma$ , see [Ca2] and [Ca3]. Note that the damping term in (2.11), which is intended to model at a phenomenological level the coupling of the electron with external light ([NM], [SSL]), readily makes the modified von Neumann equation (2.11) time-irreversible, contrary to (2.4) or equivalently (2.8).

In this picture, and contrary to these two approaches where some “noise” is introduced in the true Schrödinger equation, the present paper deals at variance with the direct limit  $T \rightarrow \infty$  and  $L \rightarrow \infty$  in (2.4) (or equivalently  $\mathcal{T} \rightarrow \infty$ ,  $L \rightarrow \infty$  in (2.8)), in a regime which includes the low-density regime  $\mathcal{T} \sim L^{d-2}$ . We prove in Theorem 1 that we do not recover (2.9) in the limit.

From a purely mathematical point of view, we now wish to illustrate the reason for the qualitatively very different results obtained here on the one hand, and in [Ca2], or [Sp], [HLW], [La], [EY] on the other hand. After some easy manipulations, it is seen that the analysis of both (2.11) and (2.4) leads to considering sums of the form,

$$F(L, \alpha) := \frac{1}{L^{2d}} \sum_{(n,p) \in \mathbb{Z}^{2d}} \int_0^{L^d t} \exp\left(i \frac{n^2 - p^2}{L^2} s - \alpha s\right) ds \phi\left(\frac{n}{L}, \frac{p}{L}\right), \quad (2.12)$$

for some smooth test function  $\phi$ . In this language, the analysis performed in [Ca2] leads to the limit  $\lim_{\alpha \rightarrow 0} \lim_{L \rightarrow \infty} \dots$  whereas the present work deals with  $\lim_{L \rightarrow \infty} \lim_{\alpha \rightarrow 0} \dots$  (and the first limit  $\alpha \rightarrow 0$  is trivial in the latter case). It is clear on (2.12) that a competition occurs between the discreteness of the sum  $\sum_{n,p}$  which should approximate an integral over  $\mathbb{R}^{2d}$ , and the convergence of

the oscillatory term  $\int_0^{L^d t} \exp(i(n^2 - p^2)s/L^2) ds$  towards the oscillatory integral  $\int_0^{+\infty} \exp(i[\mathbf{n}^2 - \mathbf{p}^2]s) ds$ , an object which only has a meaning as a distribution in the continuous variables  $\mathbf{n}$  and  $\mathbf{p}$  in  $\mathbb{R}^d$ . In particular, the convergence of Riemann sums towards their integral counterpart is not guaranteed when dealing with distributions, and in this case the sampling may destroy the convergence towards the desired oscillatory integral. The result in [Ca2] relies on the following limit,

$$\lim_{\alpha \rightarrow 0} \lim_{L \rightarrow \infty} F(L, \alpha) = \int_{\mathbb{R}^{2d}} \int_0^{+\infty} \exp(i[\mathbf{n}^2 - \mathbf{p}^2]s) \phi(\mathbf{n}, \mathbf{p}) ds d\mathbf{n} d\mathbf{p}, \quad (2.13)$$

as formally expected. However, the key of the present paper lies in proving (Theorem 2) the existence of an explicitly computable measure  $d\mu$  supported on the set  $\mathbf{n}^2 = \mathbf{p}^2$ , such that,

$$\lim_{L \rightarrow \infty} \lim_{\alpha \rightarrow 0} \frac{1}{L^{d-2}} F(L, \alpha) = \int_{\mathbb{R}^{2d}} \phi(\mathbf{n}, \mathbf{p}) d\mu(\mathbf{n}, \mathbf{p}). \quad (2.14)$$

This result (2.14) proves that the sampling of size  $1/L$  in  $n$  and  $p$  in (2.12) is somehow too crude to converge towards the natural limit (2.13). Both limits (2.13) and (2.14) answer a question posed in a physical context in [Co]. The fact that the

limits (2.13) and (2.14) differ is the very reason for the diverging results established in [Ca2] on the one hand, and here on the other hand. In the stochastic case, the phase  $n^2 - p^2$  appearing in (2.12) is somehow randomized, so that again a result of the kind (2.13) may be used.

Technically speaking, we wish to add that the exact value of the measure  $d\mu$  depends on the asymptotic behaviour of the cardinality of the set  $\{n \in \mathbb{Z}^d, \text{ s.t. } n^2 = A\}$  when  $A \rightarrow \infty$  ( $A \in \mathbb{N}$ ), as well as on the asymptotic repartition of the unitary vectors  $n/|n|$  when  $n^2 = A$  and  $A \rightarrow \infty$ . The latter asymptotics is studied independently in [CP], and it turns out that the analysis encounters deep difficulties in dimensions  $d = 3$  and  $4$ , while it remains much easier in dimensions  $d \geq 5$ .

### 2.3 Statement of the main Theorems

We now quote the statement of the main results of the present paper. In order to do so, we need to formulate an important assumption,

**(A)** There exists a  $\delta_0(d) \in ]0, 1]$  such that for any  $0 < \delta < \delta_0(d)$ , for any  $l \geq 1, l \in \mathbb{N}$ , the following limit exists,

$$\gamma_{l,d} := \lim_{A \rightarrow \infty} \frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left( \frac{\#\{n \in \mathbb{Z}^d \text{ s.t. } n^2 = B\}}{B^{\frac{d}{2}-1}} \right)^l.$$

In a less essential way, we may further assume the following bound,

**(A')** There exists a constant  $C(d)$ , depending on  $d$ , so that,

$$\gamma_{l,d} \leq C(d)^l.$$

The assumptions **(A)** and **(A')** are easily proved true for dimensions  $d \geq 5$ , and  $\delta_0(d) = 1$  in this case, see Lemma 4. In dimension  $d = 4$ , we are able to prove that the quantity involved in **(A)** is bounded independently of  $A$  for any  $\delta < \delta_0(4) = 1$ , hence the existence of a limit up to extracting a subsequence in  $A$ , see Lemma 5. However, the bound on  $\gamma_{l,4}$  which we are able to prove is of the form  $(Cl)^l$  in this case. In dimension  $d = 3$ , we are not able to prove **(A)**, which is thus a conjecture in this case (except in the special case  $l = 1$  where the estimate is easy). Needless to say, the bound **(A')** is also out of reach when  $d = 3$ . However, we have tested that the sequence in  $A$  involved in **(A)** converges *numerically* in a satisfactory way for various values of  $l$  when  $d = 3$ . Also, when  $d = 3$  or  $d = 4$ , it seems numerically plausible that the behaviour stated in **(A')** is realised. Note that the independence of  $\gamma_{l,d}$  upon  $\delta$  is natural since once the limit exists for some  $\delta > 0$ , it also exists for any  $\delta' < \delta$ , and the limit is the same.

Our main statement is now the following,

**Theorem 1** Let  $\rho(t, n, p)$  be the solution to (2.8) with initial datum given by (2.5). Assume that both  $\widehat{V}(\mathbf{n})$  and  $\rho^0(\mathbf{n})$  are smooth profiles in  $\mathcal{S}(\mathbb{R}^d)$  with  $d \geq 3$ . Define the distribution,

$$\rho_I(t, \mathbf{n}, \mathbf{p}) := \sum_{(n,p) \in \mathbb{Z}^{2d}} \exp(i\mathcal{T}t[n^2 - p^2]) \rho(t, n, p) \delta(\mathbf{n} - \frac{n}{L}) \delta(\mathbf{p} - \frac{p}{L}). \quad (2.15)$$

Take a smooth test function  $\Phi(\mathbf{n}, \mathbf{p}) \in C_c^\infty(\mathbb{R}^{2d})$  and consider the duality product,

$$\langle \rho_I(t), \Phi \rangle := \int_{\mathbb{R}^{2d}} \rho_I(t, \mathbf{n}, \mathbf{p}) \Phi(\mathbf{n}, \mathbf{p}) \, d\mathbf{n} \, d\mathbf{p}. \quad (2.16)$$

Then,

(i) the sequence  $\langle \rho_I(t), \Phi \rangle$  admits the power expansion,

$$\langle \rho_I(t), \Phi \rangle = \sum_{\substack{l \in \mathbb{N} \\ l' \in \mathbb{N}}} (-i\Lambda)^l (+i\Lambda)^{l'} \mathcal{Q}_{l,l'}(t) = \sum_{s \in \mathbb{N}} (i\Lambda)^s \sum_{l+l'=s} (-1)^l \mathcal{Q}_{l,l'}(t), \quad (2.17)$$

where the last sum  $\sum_{l+l'=s} \dots$  is finite for any  $s \geq 0$ , and the terms  $\mathcal{Q}_{l,l'}(t)$  depend upon  $\mathcal{T}$  and  $L$ , but they are independent of  $\Lambda$ . Their explicit value is given in (4.7) below. The above series converges for any  $\Lambda \in \mathbb{R}$ , given any fixed value of  $\mathcal{T}$  and  $L$ .

(ii) If we further assume **(A)**, the power series in (2.17) converges term-by-term towards the following limiting power series,

$$\langle \rho_I(t), \Phi \rangle \rightarrow \langle \rho_I^\infty(t), \Phi \rangle := \sum_{\substack{l \in \mathbb{N} \\ l' \in \mathbb{N}}} (-i\Lambda)^l (+i\Lambda)^{l'} \mathcal{Q}_{l,l'}^\infty(t), \quad (2.18)$$

as  $L$  and  $\mathcal{T}$  go to infinity in the regime (2.7). The value of the quantity  $\mathcal{Q}_{l,l'}^\infty(t)$  is given below in (5.1). The series in (2.18) converges for any  $\Lambda \in \mathbb{R}$  under assumption **(A')**.

(iii) Formulae (5.1) and (2.18) define, for any value of time  $t$ , a distribution (actually: a measure)  $\rho_I^\infty(t, \mathbf{n}, \mathbf{p})$ , which can be seen as the weak-limit of  $\rho_I(t, \mathbf{n}, \mathbf{p})$ . This distribution is invariant under the transformation,

$$t \mapsto -t, \quad i \mapsto -i. \quad (2.19)$$

In particular, the dependence of  $\rho_I^\infty(t)$  upon time  $t$  is reversible.

**Remark 1** Note that the above Theorem has several restrictions. **(a)** Firstly, it is restricted to the assumptions **(A)** respectively **(A')**, which is a restriction only for the dimension  $d = 3$ , respectively  $d = 3$  and 4. **(b)** Secondly, the convergence of the distribution  $\rho_I$  which we are able to prove here only holds as a *term by term* convergence of the power expansion (2.17). Though the limiting power series

turns out to define an analytic function of  $\Lambda$  as well (at least under assumption **(A')**), we are not able to prove satisfactory uniform estimates with respect to  $L$  and  $\mathcal{T}$  (see however (5.15) below). **(c)** The last restriction lies in the fact that our result only holds when the electron evolves in a dilated cube whose lengths in the different directions of space are rationally *dependent*, a highly *non-generic* situation. Indeed, the generic case of a cube with rationally independent lengths cannot be treated by the present analysis, due to both the appearance of small denominator problems in this case, see Remark 6 below, and to the fact that the statement analogous to Theorem 2 is false in this case. Note however that such a restriction is natural, since we aim at exhibiting a non-convergence result towards a Boltzmann equation, a result which is itself non-generic.  $\square$

**Remark 2** As one sees on the formulation of Theorem 1, the method of proof proposed in the present paper is based on the explicit computation of the value at time  $t$  of the solution  $\rho(t)$  to (2.8), in terms of the initial datum  $\rho^0$ . We obtain a series expansion (2.17), and we pass to the limit on the explicit formulae. This is a standard procedure in the context of the convergence towards “Boltzmann-like” equations, see [CIP], [BGC], [Sp], [EY]. In our particular case, it turns out that the limiting dynamics, *i.e.* the limiting value  $\rho_I^\infty(t)$ , is *still* given by a series expansion stating the value of  $\rho^\infty$ , and no simple equation relates the value of  $\rho^\infty$ . This could be compared with a similar fact in the classical context, see [BGW], where the authors simply prove the non-convergence towards the natural Boltzmann equation but the actual limiting dynamics is not expressed. We do believe that a deep difficulty prevents one to pass to the limit “directly” in the particular equation (2.8) instead of its power series solution as we do here. In particular, it seems plausible that there is no constant  $\tilde{\gamma}_d$  such that  $\gamma_{l,d} = \tilde{\gamma}_d^l$ , and this makes the limiting dynamics for  $\rho^\infty$  itself already difficult to translate into a simple equation (See (2.18) and (5.1)). Another motivation for such a credo lies in the fact that the “Riemann sums with quadratic constraints”, as they naturally arise in the proof of Theorem 1 by explicit computation, cannot be treated without number theoretical arguments, and in particular the correct rescaling of these sums (see (2.20)) is dictated by the number theoretical asymptotics (2.24), an information which seems difficult to exploit when arguing “directly” on the equation (2.8).  $\square$

**Remark 3** The distribution  $\rho_I(t, \mathbf{n}, \mathbf{p})$  is called the density matrix in the interaction picture. We wish to mention that a Theorem similar to Theorem 1 holds for the diagonal part of the density matrix, namely  $f(t, \mathbf{n}) := \sum_{n \in \mathbb{Z}^d} \rho(t, n, n) \delta(\mathbf{n} - \frac{t}{L})$ .  $\square$

The above Theorem, and in particular the need for **(A)** to hold true, turn out to be a consequence of the following,

**Theorem 2** *Let  $\phi(\mathbf{k}_0, \mathbf{k}_1, \dots, \mathbf{k}_N)$  be a smooth test function in  $\mathcal{S}(\mathbb{R}^{(N+1)d})$ , with a dimension  $d \geq 3$ . Assume **(A)** holds true. Consider finally the following “Riemann sum with quadratic constraint”,*

$$I_L(\phi) := \frac{1}{L^{d+N(d-2)}} \sum_{(k_0, \dots, k_N) \in \mathbb{Z}^{(N+1)d}} \phi\left(\frac{k_0}{L}, \dots, \frac{k_N}{L}\right) \mathbf{1}[k_0^2 = \dots = k_N^2]. \quad (2.20)$$

Then, as  $L \rightarrow \infty$ ,  $I_L(\phi)$  converges, and its explicit limit is,

$$\lim_{L \rightarrow \infty} I_L(\phi) = 2\gamma_{N+1,d} \int_{\theta=0}^{+\infty} \int_{(\mathbb{S}^{d-1})^{N+1}} \theta^{(N+1)(d-2)+1} \phi(\theta \mathbf{k}_0, \theta \mathbf{k}_1, \dots, \theta \mathbf{k}_N) d\theta d\sigma(\mathbf{k}_0) \dots d\sigma(\mathbf{k}_N). \quad (2.21)$$

Here,  $d\sigma$  denotes the Euclidean measure of the sphere  $\mathbb{S}^{d-1}$ , normalized with  $d\sigma(\mathbb{S}^{d-1}) = 1$ .

**Remark 4** As we shall see, Theorem 2 is a consequence of the following Theorem, proved in [CP] (See [Lab] for previous results): for any domain  $\Omega \subset \mathbb{S}^{d-1}$ , measurable with respect to the euclidian surface measure  $d\sigma$ , and for any dimension  $d \geq 5$ , the following asymptotics holds,

$$\frac{\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = A \text{ and } n/|n| \in \Omega\}}{\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = A\}} \sim_{A \rightarrow \infty} d\sigma(\Omega). \quad (2.22)$$

In fact, formula (2.22) still holds true *in average* for the dimensions  $d = 4$  and  $d = 3$  as well, in the sense that,

$$\frac{1}{1+h} \sum_{B=A}^{A+h} \frac{\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = B \text{ and } n/|n| \in \Omega\}}{\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = B\}} \sim_{A \rightarrow \infty} d\sigma(\Omega), \quad (2.23)$$

up to choosing  $h = A^\varepsilon$  for any small  $\varepsilon > 0$  when  $d = 4$ , and  $h = A^{1/4+\varepsilon}$  when  $d = 3$ .  $\square$

**Remark 5** Before turning to the proofs of all these results, we wish to justify now the exact scaling needed in (2.20), and recall some important facts from number theory. These will be of constant use below.

Without the constraint  $k_0^2 = \dots = k_N^2$ , the correct normalization of the Riemann sum is given by the prefactor  $1/L^{(N+1)d}$  instead of  $1/L^{d+N(d-2)}$ . The quadratic constraint modifies the prefactor because the number of  $(N+1)$ -tuples of modulus  $\sim L$  satisfying the constraint, is of the order  $L^{d+N(d-2)}$  rather than  $L^{(N+1)d}$ . This point is easily seen since, roughly speaking, the cardinality  $\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = A\}$  is of the order  $A^{\frac{d}{2}-1}$ . We make this point more precise below.

It is well known (see [Gr], [Va]) that,

$$\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = A\} \sim_{A \rightarrow \infty} \frac{\Gamma(3/2)^d}{\Gamma(d/2)} \mathfrak{S}(A) A^{\frac{d}{2}-1}, \quad (2.24)$$

(when  $d \geq 3$ ), and  $\mathfrak{S}(A)$  is the so-called singular series, defined as,

$$\mathfrak{S}(A) := \sum_{q \geq 1} \sum_{\substack{a=1 \\ \gcd(a,q)=1}}^q \left( \frac{S(q,a)}{q} \right)^d \exp\left(-2i\pi \frac{aA}{q}\right), \quad (2.25)$$

where we use the notation,

$$S(q, a) := \sum_{m=1}^q \exp\left(2i\pi \frac{am^2}{q}\right). \quad (2.26)$$

By a standard estimate on Gauss' sums (see [Gr]), we have  $|S(q, a)| \leq Cq^{1/2}$ , for some constant  $C \geq 0$ , so that the series over  $q$  in (2.25) defining  $\mathfrak{S}(A)$  has a general term which is upper-bounded by  $1/q^{\frac{d}{2}-1}$ , and the series absolutely converges in dimensions  $d \geq 5$ . The convergence of this series is much more delicate in dimension  $d = 4$  and even more delicate when  $d = 3$ , which explains the separate treatment of these two dimensions in this paper.

Now  $\mathfrak{S}(A)$  is roughly speaking a quantity of the order 1, a statement that assumption **(A)** translates in a more quantitative way. In particular, we wish to mention that, as is well-known ([Gr]), in dimensions  $d \geq 5$ , there are positive constants  $c_0(d)$  and  $c_1(d)$  such that for any  $A \in \mathbb{N}$ ,

$$0 < c_0(d) \leq \mathfrak{S}(A) \leq c_1(d) < \infty. \quad (2.27)$$

In dimensions  $d = 4$  and  $d = 3$ , this estimate becomes wrong as such, and one can only prove (see [Gr]),

$$0 \leq \mathfrak{S}(A) \leq c_2(\varepsilon, d)A^\varepsilon, \quad (2.28)$$

for some constant  $c_2(\varepsilon, d)$  depending on  $\varepsilon > 0$  and  $d = 3$  or  $4$  (this estimate is not optimal yet, see [Gr] for refined estimates). Hence  $\mathfrak{S}(A)$  can be arbitrarily small (it may vanish) or as large as  $A^\varepsilon$  in dimensions 3 and 4. We refer to [Gr] and [Va] for these results.

Summarizing, we end this remark by stating the following bound,

$$\#\{n \in \mathbb{Z}^d \text{ such that } n^2 = A\} \leq C(\varepsilon, d)A^{\frac{d}{2}-1+\varepsilon}, \quad (2.29)$$

for some constant  $C(\varepsilon, d)$  depending on  $\varepsilon > 0$  and  $d \geq 3$ , and one can choose  $\varepsilon = 0$  when  $d \geq 5$ . This is an obvious consequence of the above estimates. We shall make repeated use of this estimate below.  $\square$

## 2.4 Organisation of the paper, notations

The paper is organised as follows:

**1-** In Section 3, we present a simple computation which is a model for all the computations appearing in the present paper. We explain on this computation the main features of our analysis, and the proof of Theorem 1 simply uses in a general setting the ideas of Section 3.

**2-** In Section 4, we explicitly compute the solution  $\rho(t, n, p)$  to (2.8), for any finite value of the scaling parameters  $L$  and  $\mathcal{T}$ .

**3-** The explicit formula obtained in Section 4 involves a factor called  $H_l$  (see (4.1)) which is some integral over the variables  $t_1, \dots, t_l$  of an oscillatory function of the form  $\exp(i\mathcal{T}[\omega_1 t_1 + \dots + \omega_l t_l])$ , and the  $\omega_i$ 's are integers. By the

Riemann-Lebesgue Lemma, it is clear that this kind of factor goes to zero *at least* like  $1/\mathcal{T}$  when *one* of the  $\omega_i$ 's is non-zero. It is a key argument in the present paper that we can prove a much more refined estimate stating (very roughly) that  $H_l$  goes like  $1/\mathcal{T}^r$  when  $r$  terms amongst the  $\omega_i$ 's are nonzero (see (5.9) for the exact estimate), so that we can relate the size of  $H_l$  and the number of non-zero  $\omega_i$ 's. The corresponding precise analysis is performed in Subsection 5.2.

**4-** Armed with the bounds of Subsection 5.2, we prove in Subsection 5.3.2 that the “non-resonant” terms in the explicit formula for  $\rho(t, n, p)$  (corresponding roughly to the case  $n^2 \neq p^2$  in (2.8)) go to zero like  $(L^\varepsilon \log L)/\mathcal{T}$  in the regime (2.7), for any  $\varepsilon > 0$ . This is based upon a very careful analysis of the “number of non-zero  $\omega_i$ 's” in factors involving the function  $H_l$ , and the key difficulty lies in keeping precise track of the homogeneity of our formulae in the scaling parameters  $L$  and  $\mathcal{T}$ . Then we compute in Subsection 5.3.3 the limit of the remaining “resonant” terms (corresponding roughly to the case  $n^2 = p^2$  in (2.8)), by making use of the convergence of sums of the form (2.20). This ends the proof of Theorem 1.

**5-** In Section 6, we prove Theorem 2 upon the basis of the results (2.22) and (2.23) proved in [CP]. This uses assumption **(A)**.

**6-** In Section 7, we prove the assumptions **(A)** and **(A')** in the cases  $d \geq 5$ , as well as a weaker form of **(A)** and **(A')** when  $d = 4$ .

## Notations

The following notational conventions are used.

**(i)** In the sequel,  $C(a, b, \dots)$  denotes any positive constant depending upon the parameters  $a, b, \dots$ . In most cases, the important point for us is to check that  $C$  does not depend upon the scaling parameters  $L$  and  $\mathcal{T}$ . However, these various constants may depend upon the dimension  $d$ , the profiles  $\rho^0$  and  $\widehat{V}$  without explicitly emphasizing the dependence upon these three parameters.

**(ii)** In the sequel, the letters  $m, n, p, k, k_1, k_2, \dots, j, j_1, j_2, \dots$ , always denote integers in  $\mathbb{Z}^d$ , and they are possibly indexed by integers in  $\mathbb{N}$ . The symbol  $\sum_{n,p,j,\dots}$  always denotes the sum extended to all integers  $n, p, k, j, \dots$  in  $\mathbb{Z}^d$ .

**(iii)** For any integer  $m$ , the symbol  $\llbracket 1, m \rrbracket$  denotes the set  $[1, m] \cap \mathbb{Z}$ .

**(iv)** An inequality of the form  $\dots \leq C(\varepsilon)A^{1-\varepsilon}$  always means that for any small enough  $\varepsilon > 0$ , there exists a constant  $C(\varepsilon)$  such that the inequality is satisfied. In particular, we may sometimes replace  $x^{2\varepsilon}$  by  $x^\varepsilon$  in a chain of inequalities without further comment.

**(v)** For any  $\mathbf{n} \in \mathbb{R}^d$ , we use the notations,

$$\langle \mathbf{n} \rangle := (1 + \mathbf{n}^2)^{1/2}, \quad \text{and} \quad \mathbf{n}^2 := \mathbf{n}_1^2 + \dots + \mathbf{n}_d^2. \quad (2.30)$$

**(vi)** Throughout the paper,  $d\sigma$  denotes the Euclidean surface measure over the sphere  $\mathbb{S}^{d-1}$ , normalized by  $d\sigma(\mathbb{S}^{d-1}) = 1$ .

**(vii)** We shall make repeated use of the following easy relations: for any smooth and sufficiently decaying function  $\phi$  defined over  $\mathbb{R}^N$ , and for any  $L \geq 1$ , we have,

$$\left| \frac{1}{L^N} \sum_{k \in \mathbb{Z}^N} \phi\left(\frac{k}{L}\right) \right| \leq C(\phi) \quad , \quad \frac{1}{L^N} \sum_{k \in \mathbb{Z}^N} \phi\left(\frac{k}{L}\right) \xrightarrow{L \rightarrow \infty} \int_{\mathbb{R}^N} \phi(\mathbf{k}) d\mathbf{k}. \quad (2.31)$$

### 3 A model computation

Before turning to the asymptotic analysis of (2.8) in the regime (2.7), we first present a model computation containing the main features of the present analysis.

As it will be clear below, the study of (2.8) typically requires to characterize the asymptotic behaviour of the model term,

$$S_{L,\mathcal{T}}(\phi) := \frac{1}{L^{d+(d-2)}} \sum_{(n,p) \in \mathbb{Z}^{2d}} \phi\left(\frac{n}{L}, \frac{p}{L}\right) \int_{s=0}^t \exp(i\mathcal{T}[n^2 - p^2]s) ds, \quad (3.1)$$

for some smooth and compactly supported test function  $\phi(\mathbf{n}, \mathbf{p})$ , say (see also (2.12), (2.13) and (2.14)). The important point to notice is that this sum, though formally similar to a Riemann sum, *is not* normalized like a usual Riemann sum. However, we prove below that this term converges as  $\mathcal{T}$  and  $L$  go to infinity in the regime (2.7). The idea is that the normalization by  $L^{-(2d-2)}$  is correct over the resonant set  $n^2 = p^2$  in view of Theorem 2. Outside the resonant set, i.e. when  $n^2 \neq p^2$ , the sum is apparently incorrectly normalized, but the factor  $\mathcal{T}[n^2 - p^2]$  in the phase turns out to both restore the correct normalization upon computing the integral of the complex exponential in (3.1), and to give the desired concentration on the set  $n^2 = p^2$  as  $\mathcal{T} \rightarrow \infty$ . These three features are the key arguments allowing us to prove Theorem 1 in Section 5. In particular, a key step in the present model computation lies in explicitly computing the integral  $\int_0^t \exp(i\mathcal{T}[n^2 - p^2]s) ds$  to restore the correct normalization of the sum (3.1), and we wish to mention that this step “simply” has to be replaced by the bound (5.9) in the general case as treated in Section 5.

Now, we come to the study of  $S_{L,\mathcal{T}}$ . It is first natural to split  $S_{L,\mathcal{T}}(\phi)$  into a non-resonant contribution, for which  $n^2 \neq p^2$  in (3.1), and a resonant contribution, for which  $n^2 = p^2$ , as follows,

$$\begin{aligned} S_{L,\mathcal{T}} &= \frac{1}{L^{d+(d-2)}} \sum_{\substack{(n,p) \in \mathbb{Z}^{2d} \\ n^2 \neq p^2}} \cdots + \frac{1}{L^{d+(d-2)}} \sum_{\substack{(n,p) \in \mathbb{Z}^{2d} \\ n^2 = p^2}} \cdots \\ &=: S_{L,\mathcal{T}}^{(1)}(\phi) + S_{L,\mathcal{T}}^{(2)}(\phi). \end{aligned}$$

*First step: study of the non resonant term*

We first prove the bound,

$$|S_{L,\mathcal{T}}^{(1)}(\phi)| \leq C(\varepsilon) \frac{L^\varepsilon \log L}{\mathcal{T}},$$

for some constant  $C(\varepsilon)$  depending on  $\varepsilon > 0$ , where  $\varepsilon = 0$  is allowed when  $d \geq 5$ , and we recall,

$$S_{L,\mathcal{T}}^{(1)}(\phi) = \frac{1}{L^{d+(d-2)}} \sum_{n^2 \neq p^2} \phi\left(\frac{n}{L}, \frac{p}{L}\right) \int_{s=0}^t \exp(i\mathcal{T}[n^2 - p^2]s) ds.$$



The analogous bound in the general case is (5.13) below.

Decomposing the sum  $\sum_{n^2 \neq p^2}$  into a sum over the different values of the difference  $n^2 - p^2 := \omega \in \mathbb{Z}^*$ , we readily obtain,

$$|S_{L,\mathcal{T}}^{(1)}(\phi)| \leq \frac{1}{L^{d+(d-2)}} \sum_{\omega \in \mathbb{Z}^*} \sum_{n^2 - p^2 = \omega} \left| \phi\left(\frac{n}{L}, \frac{p}{L}\right) \int_{s=0}^t \exp(i\mathcal{T}\omega s) ds \right|,$$

hence, by explicit computation of the integral in  $s$ ,

$$|S_{L,\mathcal{T}}^{(1)}(\phi)| \leq \frac{C}{\mathcal{T} L^{d+(d-2)}} \sum_{\omega \in \mathbb{Z}^*} \frac{1}{|\omega|} \sum_{n^2 - p^2 = \omega} \left| \phi\left(\frac{n}{L}, \frac{p}{L}\right) \right|.$$

Now, we first use the fact that  $\phi$  has compact support, so that the above sum is actually restricted to bounded values of  $n^2/L^2$  and  $p^2/L^2$  hence, say,  $|\omega| \leq L^2$  and  $n^2 \leq L^2$  up to a multiplicative constant. This gives,

$$\begin{aligned} |S_{L,\mathcal{T}}^{(1)}(\phi)| &\leq \frac{C}{\mathcal{T} L^{d+(d-2)}} \\ &\times \sum_{1 \leq |\omega| \leq L^2} \frac{1}{|\omega|} \#\{(n, p) \in \mathbb{Z}^{2d} \text{ s. t. } n^2 \leq L^2, p^2 = n^2 - \omega\}. \end{aligned} \quad (3.2)$$

Secondly, we make use of the fundamental result (see (2.29)),

$$\#\{p \in \mathbb{Z}^d \text{ s.t. } p^2 = n^2 - \omega\} \leq C(\varepsilon) |n^2 - \omega|^{\frac{d}{2} - 1 + \varepsilon}, \quad (3.3)$$

in any dimension  $d \geq 3$ . Hence, in view of  $|\omega| \leq L^2$  and  $n^2 \leq L^2$ , we obtain,

$$\#\{p \in \mathbb{Z}^d \text{ s.t. } p^2 = n^2 - \omega\} \leq C(\varepsilon) L^{d-2+\varepsilon},$$

so that,

$$|S_{L,\mathcal{T}}^{(1)}(\phi)| \leq \frac{C(\varepsilon)}{\mathcal{T} L^{d+(d-2)}} \sum_{1 \leq |\omega| \leq L^2} \frac{1}{|\omega|} \times L^d \times L^{d-2+\varepsilon} \leq C(\varepsilon) \frac{L^\varepsilon \log L}{\mathcal{T}} \rightarrow 0,$$

and (3.2) is proved. Note that the factor  $\log L$  in (3.2) is directly related to the logarithmic divergence of the harmonic series.

**Remark 6** We heavily used that the difference  $n^2 - p^2$  belongs to  $\mathbb{Z}$ , hence no small denominator problems occur here. This is the reason why the analysis in this paper cannot be applied in the case where the initial Schrödinger equation is posed on a cube with rationally independent sides: in this case indeed, the relation  $\omega = n^2 - p^2$  is replaced by  $\omega = \sum_{i=1}^d \lambda_i (n_i^2 - p_i^2)$  for some rationally independent  $\lambda_i$ 's in  $\mathbb{R}$ , and one cannot use the implication  $\omega \neq 0 \Rightarrow |\omega| \geq 1$  anymore. Anyhow, the numbering (3.3) has to be adapted in the rationally independent case.  $\square$

*Second step: study of the resonant term*

It is defined as,

$$S_{L,\mathcal{T}}^{(2)}(\phi) = \frac{t}{L^{d+(d-2)}} \sum_{n^2=p^2} \phi\left(\frac{n}{L}, \frac{p}{L}\right). \quad (3.4)$$

We are thus led to studying ‘‘Riemann sums with quadratic constraint’’ as in (3.4) above, and Theorem 2 together with (3.2) thus give in the regime (2.7),

$$\begin{aligned} \lim_{L, T \rightarrow \infty} S_{L, T}(\phi) &= \lim_{L, T \rightarrow \infty} S_{L, T}^{(2)}(\phi) \\ &= 2\gamma_{2, d} \int_{\theta=0}^{+\infty} \int_{\mathbb{S}^{2(d-1)}} \theta^{2(d-2)+1} \phi(\theta \mathbf{n}, \theta \mathbf{p}) d\theta d\sigma(\mathbf{n}) d\sigma(\mathbf{p}) . \end{aligned} \quad (3.5)$$

The analysis of (3.1) is complete.

## 4 Proof of Theorem 1, part (i): explicit solution to the von Neumann equation (2.8)

In this section, we explicitly compute the solution to (2.8). In order to do so, we first need the following,

### Definition 1

(i) For any  $(\omega_1, \dots, \omega_l) \in \mathbb{R}^l$ , we define the following quantity,

$$H_l(\omega_1, \dots, \omega_l) := \int_{s_1=0}^t \int_{s_2=0}^{t-s_1} \dots \int_{s_l=0}^{t-s_1-\dots-s_{l-1}} \exp(i\mathcal{T}[\omega_1 s_1 + \dots + \omega_l s_l]) . \quad (4.1)$$

Explicit formulae for  $H_l$  are given in (5.5) and (5.9) below.

(ii) For any values of  $(k_0, k_1, \dots, k_l) \in \mathbb{Z}^{(l+1)d}$ , we define,

$$\mathcal{V}_l \left( \frac{k_0}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{k_l}{L} \right) := \widehat{\mathcal{V}} \left( \frac{k_0 - k_1}{L} \right) \widehat{\mathcal{V}} \left( \frac{k_1 - k_2}{L} \right) \dots \widehat{\mathcal{V}} \left( \frac{k_{l-1} - k_l}{L} \right) . \quad (4.2)$$

**Remark 7** We readily state some easy bounds on  $H_l$  and  $\mathcal{V}_l$ . Firstly, the following bound on  $H_l$  is trivial,

$$|H_l(\omega_1, \dots, \omega_l)| \leq \frac{|t|^l}{l!} . \quad (4.3)$$

Secondly, due to the assumption  $\mathcal{V} \in \mathcal{S}(\mathbb{R}^d)$ , it follows that for any  $M \geq 0$ , there exists a constant  $C(M)$  such that,

$$|\widehat{\mathcal{V}}(\mathbf{n})| \leq C(M) \langle \mathbf{n} \rangle^{-M} . \quad (4.4)$$

In particular we may upper-bound  $\mathcal{V}_l$  as,

$$\left| \mathcal{V}_l \left( \frac{k_0}{L}, \frac{k_1}{L}, \dots, \frac{k_l}{L} \right) \right| \leq C(M)^l \left\langle \frac{k_0 - k_1}{L} \right\rangle^{-M} \dots \left\langle \frac{k_{l-1} - k_l}{L} \right\rangle^{-M} , \quad (4.5)$$

for any  $M \geq 0$ . We mention that the following weaker bound is also of interest,

$$\left| \mathcal{V}_l \left( \frac{k_0}{L}, \frac{k_1}{L}, \dots, \frac{k_l}{L} \right) \right| \leq C(M)^l \left\langle \frac{k_0^2 - k_1^2}{L^2} \right\rangle^{-M} \dots \left\langle \frac{k_{l-1}^2 - k_l^2}{L^2} \right\rangle^{-M} . \quad (4.6)$$

□

With these notations, we are in position to state the,

**Proposition 1** *Part (i) of Theorem 2 holds true up to defining the quantities,*

$$\begin{aligned} \mathcal{Q}_{l,l'}(t) &= \frac{1}{L^{d+(l+l')(d-2)}} \sum_{m,n,p,k_1,\dots,k_{l-1},j_1,\dots,j_{l'-1}} \exp(i\mathcal{T}t[n^2 - p^2]) \\ &\times H_l(m^2 - n^2, m^2 - k_1^2, \dots, m^2 - k_{l-1}^2) \\ &\times H_{l'}(p^2 - m^2, j_1^2 - m^2, \dots, j_{l'-1}^2 - m^2) \\ &\times \mathcal{V}_l\left(\frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L}\right) \mathcal{V}_l^*\left(\frac{p}{L}, \frac{j_1}{L}, \dots, \frac{j_{l'-1}}{L}, \frac{m}{L}\right) \rho^0\left(\frac{m}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right), \end{aligned} \quad (4.7)$$

when  $l \geq 1$  and  $l' \geq 1$ . This definition has to be extended when  $l = 0$ ,  $l' \geq 1$  by,

$$\begin{aligned} \mathcal{Q}_{0,l'}(t) &= \frac{1}{L^{d+l'(d-2)}} \sum_{n,p,j_1,\dots,j_{l'}} \exp(i\mathcal{T}t[n^2 - p^2]) \\ &\times H_{l'}(p^2 - n^2, j_1^2 - n^2, \dots, j_{l'}^2 - n^2) \\ &\times \mathcal{V}_l^*\left(\frac{p}{L}, \frac{j_1}{L}, \dots, \frac{j_{l'-1}}{L}, \frac{n}{L}\right) \rho^0\left(\frac{n}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right), \end{aligned} \quad (4.8)$$

and similarly when  $l \geq 1$ ,  $l' = 0$ . Also, when  $l = l' = 0$ , we have to define,

$$\mathcal{Q}_{0,0}(t) = \frac{1}{L^d} \sum_n \rho^0\left(\frac{n}{L}\right) \Phi\left(\frac{n}{L}, \frac{n}{L}\right). \quad (4.9)$$

**Remark 8** For fixed values of the scaling parameters  $\mathcal{T}$  and  $L$ , the series in  $\Lambda$ ,  $\sum_{l \in \mathbb{N}, l' \in \mathbb{N}} (-i\Lambda)^l (+i\Lambda)^{l'} \mathcal{Q}_{l,l'}(t)$ , involved in (2.17) is easily seen to converge for any  $\Lambda \in \mathbb{R}$ . Indeed, when  $l \geq 1$  and  $l' \geq 1$  say, we may upper bound  $\mathcal{Q}_{l,l'}(t)$  as,

$$\begin{aligned} \left| \mathcal{Q}_{l,l'}(t) \right| &\leq C(\Phi)^{l+l'} \frac{|t|^{l+l'}}{l! l'} \times \frac{1}{L^{d+(l+l')(d-2)}} \\ &\sum_{m,n,p,k_1,\dots,k_{l-1},j_1,\dots,j_{l'-1}} \left\langle \frac{n - k_1}{L} \right\rangle^{-(d+1)} \left\langle \frac{k_1 - k_2}{L} \right\rangle^{-(d+1)} \dots \left\langle \frac{k_{l-1} - m}{L} \right\rangle^{-(d+1)} \\ &\left\langle \frac{p - j_1}{L} \right\rangle^{-(d+1)} \left\langle \frac{j_1 - j_2}{L} \right\rangle^{-(d+1)} \dots \left\langle \frac{j_{l'-1} - m}{L} \right\rangle^{-(d+1)} \left\langle \frac{m}{L} \right\rangle^{-(d+1)} \\ &\leq \frac{C(\Phi, t)^{l+l'} L^{2(l+l')}}{l! l'}, \end{aligned} \quad (4.10)$$

where we used successively (4.3), (4.5) for  $M = d + 1$ ,  $|\rho^0(\mathbf{n})| \leq C(\mathbf{n})^{-(d+1)}$ ,  $|\Phi(\mathbf{n}, \mathbf{p})| \leq C(\Phi)$ , and (2.31) with  $N = d(l + l' + 1)$ .

Clearly, the bound (4.10) implies that for fixed values of  $L$  and  $\mathcal{T}$ , the series in (2.17) behaves like  $C(L, \mathcal{T}, t, \Phi)^{l+l'} |\Lambda|^{l+l'} (l!)^{-1} (l')^{-1}$ , hence the convergence. We mention in passing that another estimate on  $\mathcal{Q}_{l,l'}(t)$  is available, see (5.15), which is uniform in  $\mathcal{T}$  and  $L$ , but it grows with  $l$  and  $l'$ .  $\square$

**Proof of Proposition 1** The proof is given in several steps.

*First step: factorizing the solution to (2.8)*

Let us define the auxiliary function,

$$g(t, n, p) := \exp(i\mathcal{T}t[n^2 - p^2]) \rho(t, n, p), \quad (4.11)$$

where  $\rho$  is the solution to (2.8). One easily checks from (2.8) and (4.11) that  $g(t, n, p)$  satisfies,

$$\begin{aligned} \partial_t g(t, n, p) = & -i \frac{\Lambda}{L^{d-2}} \sum_{k \in \mathbb{Z}^d} \left\{ \exp(i\mathcal{T}t[n^2 - k^2]) \widehat{V}\left(\frac{n-k}{L}\right) g(t, k, p) \right. \\ & \left. - \exp(i\mathcal{T}t[k^2 - p^2]) \widehat{V}\left(\frac{k-p}{L}\right) g(t, n, k) \right\}, \end{aligned} \quad (4.12)$$

with initial data given by (2.5) as well. Now it is a standard procedure to observe that the solution  $g(t, n, p)$  can be factorized under the form,

$$g(t, n, p) = \sum_{m \in \mathbb{Z}^d} \psi_m(t, n) \psi_m(t, p)^*, \quad (4.13)$$

where the wave functions  $\psi_m(t, n)$  satisfy,

$$\partial_t \psi_m(t, n) = -i \frac{\Lambda}{L^{d-2}} \sum_k \exp(i\mathcal{T}t[n^2 - k^2]) \widehat{V}\left(\frac{n-k}{L}\right) \psi_m(t, k), \quad (4.14)$$

with initial data given by,

$$\psi_m(t, n)|_{t=0} = \frac{1}{L^{\frac{d}{2}}} \sqrt{\rho^0\left(\frac{m}{L}\right)} \mathbf{1}[n = m]. \quad (4.15)$$

The proof of (4.13) is very simple: from (4.14), it is obvious that the right-hand-side of (4.13) satisfies (2.8), with initial data given by (2.5) thanks to (4.15). We conclude using the fact that the solution to (2.8) for a given initial data is unique. The problem of computing the solution  $\rho(t, n, p)$  to the von Neumann equation (2.8) with initial data (2.5) is thus reduced to computing the wave functions  $\psi_m(t, n)$  ( $m \in \mathbb{Z}^d$ ) defined above, solutions to the simpler Schrödinger equation (4.14).

*Second step: solving (4.14)*

Integrating the equation (4.14) in time and taking the initial data (4.15) into account, we readily obtain,

$$\begin{aligned} \psi_m(t, n) = & \frac{1}{L^{\frac{d}{2}}} \sqrt{\rho^0\left(\frac{m}{L}\right)} \mathbf{1}[n = m] \\ & -i \frac{\Lambda}{L^{d-2}} \int_{s=0}^t \exp(i\mathcal{T}s[n^2 - k^2]) \widehat{V}\left(\frac{n-k}{L}\right) \psi_m(s, k) ds. \end{aligned} \quad (4.16)$$

Hence, solving (4.16) iteratively, we obtain,

$$\begin{aligned} \psi_m(t, n) &= \sqrt{\rho^0\left(\frac{m}{L}\right)} \mathbf{1}[n = m] \\ &+ \sum_{l \geq 1} (-i\Lambda)^l \frac{1}{L^{\frac{d}{2} + l(d-2)}} \sum_{k_1, \dots, k_{l-1}} \int_{s_1=0}^t \int_{s_2=0}^{s_1} \cdots \int_{s_l=0}^{s_{l-1}} \\ &\exp(i\mathcal{T} s_1 [n^2 - k_1^2]) \exp(i\mathcal{T} s_2 [k_1^2 - k_2^2]) \cdots \exp(i\mathcal{T} s_l [k_{l-1}^2 - m^2]) \\ &\mathcal{V}_l\left(\frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L}\right) \sqrt{\rho^0\left(\frac{m}{L}\right)}. \end{aligned}$$

Now, we change variables,  $u_1 = t - s_1$ ,  $u_2 = t - s_1 - s_2$ ,  $\dots$ ,  $u_l = t - s_1 - \cdots - s_l$ , in the above equation. This gives,

$$\begin{aligned} \psi_m(t, n) &= \sqrt{\rho^0\left(\frac{m}{L}\right)} \mathbf{1}[n = m] \tag{4.17} \\ &+ \sum_{l \geq 1} (-i\Lambda)^l \frac{1}{L^{\frac{d}{2} + l(d-2)}} \sum_{k_1, \dots, k_{l-1}} \exp(i\mathcal{T} t [n^2 - m^2]) \mathcal{V}_l\left(\frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L}\right) \\ &\times H_l(m^2 - n^2, m^2 - k_1^2, \dots, m^2 - k_{l-1}^2) \sqrt{\rho^0\left(\frac{m}{L}\right)}. \end{aligned}$$

and the notations (4.1), (4.2) are used.

*Last step: conclusion*

Combining (4.17) and the factorization (4.13) proves Proposition 1.  $\square$

## 5 Proof of Theorem 1, parts (ii) and (iii): Limiting behaviour of the solution to (2.8)

### 5.1 Preliminaries : precise formulation of Theorem 1 and scheme of the proof

In this section we prove the following,

**Proposition 2** *Parts (ii) and (iii) of Theorem 1 hold true, where for each  $l$  and  $l'$ ,  $\mathcal{Q}_{l,l'}^\infty(t)$  admits the following value,*

$$\begin{aligned} \mathcal{Q}_{l,l'}^\infty(t) &= 2\gamma_{l+l'+1,d} \frac{t^{l+l'}}{l! l'} \int_{\theta=0}^{+\infty} \int_{\mathbb{S}^{(d-1)(l+l'+1)}} \mathcal{V}_l(\theta \mathbf{k}_0, \theta \mathbf{k}_1, \dots, \theta \mathbf{k}_{l-1}, \theta \mathbf{m}) \\ &\times \mathcal{V}_l^*(\theta \mathbf{j}_0, \theta \mathbf{j}_1, \dots, \theta \mathbf{j}_{l'-1}, \theta \mathbf{m}) \rho^0(\theta \mathbf{m}) \Phi(\theta \mathbf{k}_0, \theta \mathbf{j}_0) \tag{5.1} \\ &\times \theta^{(d-2)(l+l'+1)+1} d\theta d\sigma(\mathbf{m}) d\sigma(\mathbf{k}_0) \cdots d\sigma(\mathbf{k}_{l-1}) d\sigma(\mathbf{j}_0) \cdots d\sigma(\mathbf{j}_{l'-1}). \end{aligned}$$

*This definition is easily extended to the cases  $l = 0$  or  $l' = 0$ . The claimed invariance of  $\rho^\infty(t)$  under the transformation (2.19) is easily seen on the explicit formulae (5.1) and (2.18). The convergence of the series (2.18) under assumption **(A')** is a consequence of the easy estimate (5.2) below.*

**Remark 9** Let  $R$  be the typical size of the support of  $\Phi$ , and assume **(A')** holds true. Then we have the easy estimate,

$$|\mathcal{Q}_{i,l'}^\infty(t)| \leq \frac{C(t)^{l+l'}}{l! l'!} R^{(d-2)(l+l'+1)+2}, \quad (5.2)$$

where we used that  $|\mathcal{V}_l| \leq C^l$ .  $\square$

Clearly, Theorem 1 is completely proved once Proposition 2 is proved. On the more, in view of part (i) of Theorem 1, we only have to study the asymptotic behaviour of each term  $\mathcal{Q}_{i,l'}(t)$  (see (4.7)) as  $\mathcal{T}$  and  $L$  go to infinity, in order to prove Proposition 2.

Now, the method of proof of Proposition 2 is the following. It follows exactly the same lines as the model computation of section 3. The proof occupies the whole remainder part of the present Section (Subsections 5.2 to 5.3.3).

Firstly, we observe that the explicit formula (4.7) involves the factors  $H_l(m^2 - n^2, \dots, m^2 - k_{l-1}^2) H_{l'}(m^2 - p^2, \dots, m^2 - j_{l'-1}^2)$ . On the other hand, the definition of the function  $H_l(\omega_1, \dots, \omega_l)$  clearly indicates that  $H_l$  “concentrates” on the set  $\omega_1 = \dots = \omega_l = 0$  as  $\mathcal{T}$  goes to infinity. Our first step is thus to give precise bounds on  $H_l$  which give the desired quantitative version of this fact (subsection 5.2, estimate (5.9)).

As a consequence, the sum (4.7) is expected to concentrate on the “resonant” set, defined as,

$$\{(m, n, p, k_1, \dots, k_{l-1}, j_1, \dots, j_{l'-1}) \in \mathbb{Z}^{d(l+l'+1)} \text{ such that} \quad (5.3)$$

$$n^2 = p^2 = m^2 = k_1^2 = \dots = k_{l-1}^2 = j_1^2 = \dots = j_{l'-1}^2\}.$$

If the “non-resonant” set is defined as the complementary set to the resonant set, our second step is to prove that the asymptotic contribution of the “non-resonant” set (see the term  $\mathcal{Q}_{i,l'}^{\text{nr}}(t)$  in (5.12)) converges indeed to zero (subsection 5.3.2, estimate (5.13)). This is the most difficult task while proving proposition 2.

The problem thus reduces to compute the asymptotic contribution of the set  $m^2 = n^2 = p^2 = \dots$  in the sum (4.7) (see the term  $\mathcal{Q}_{i,l'}^{\text{res}}(t)$  in (5.11)). In other terms, we have to deal with a Riemann sum with constraint as it is considered in Theorem 2. Our third and last step thus consists in using Theorem 2 to conclude (subsection 5.3.3). The proof of Theorem 2 itself is deferred to the next section.

## 5.2 Part I of the proof: Explicit formulae and bounds for $H_l$

In this section, we first explicitly compute  $H_l$  as defined in (4.1). Then we indicate how to upper-bound the quantity  $H_l$ . The bounds obtained in this section will standly be used in the asymptotic analysis of the terms  $\mathcal{Q}_{i,l'}(t)$  performed in Subsections 5.3.2 and 5.3.3.

### 5.2.1 An explicit formula for $H_l$

We begin with the easy,

**Lemma 1** Defining  $H_l(\omega_1, \dots, \omega_l)$  as in (4.1). Also, define conventionally,

$$\omega_{l+1} := 0, \quad (5.4)$$

and consider  $H_l$  as a function of the  $(l+1)$ -tuple  $(\omega_1, \dots, \omega_l, \omega_{l+1})$ , a convention standly used in the sequel. Then, when  $\omega_j \neq \omega_k, \forall j \neq k$ , we have the following explicit formula,

$$H_l(\omega_1, \dots, \omega_l) = \sum_{k=1}^{l+1} \frac{\exp(iTt\omega_k)}{\prod_{\substack{j=1 \\ j \neq k}}^{l+1} [iT(\omega_k - \omega_j)]}. \quad (5.5)$$

### Proof of Lemma 1

We write,

$$\begin{aligned} H_l &= \int_{u_1=0}^t \dots \int_{u_{l-1}=0}^{t-u_1-\dots-u_{l-2}} \exp(iT[u_1\omega_1 + \dots + u_{l-1}\omega_{l-1}]) \\ &\quad \times \int_{u_l=0}^{t-u_1-\dots-u_{l-1}} \exp(iTu_l\omega_l) \\ &= \int_{u_1=0}^t \dots \int_{u_{l-1}=0}^{t-u_1-\dots-u_{l-2}} \exp(iT[u_1\omega_1 + \dots + u_{l-1}\omega_{l-1}]) \\ &\quad \times \frac{\exp(iT(t-u_1-\dots-u_{l-1})\omega_{l-1}) - 1}{iT\omega_l} \\ &= \frac{1}{iT\omega_l} [\exp(iTt\omega_l)H_{l-1}(\omega_1 - \omega_l, \dots, \omega_{l-1} - \omega_l) - H_{l-1}(\omega_1, \dots, \omega_{l-1})]. \end{aligned}$$

This gives a relation between  $H_l$  and  $H_{l-1}$ , and formula (5.5) follows by induction.  $\square$

### 5.2.2 Bounds on $H_l$

Using (5.5), we want to derive bounds on  $H_l$  when the  $\omega$ 's vary in  $\mathbb{Z}$ . In view of (5.5), the bound necessarily depends on the number of *different*  $\omega_i$ 's in the  $(l+1)$ -tuple  $(\omega_1, \dots, \omega_l, \omega_{l+1} := 0)$ . If  $r$  is the latter number, with  $1 \leq r \leq l+1$ , one readily hopes for a bound of the kind  $|H_l| \leq C/T^{r-1}$ . Indeed in the extreme case where  $r = l+1$  (this is a ‘‘completely non-resonant case’’),  $H_l$  should decay like  $T^{-l}$  as  $T \rightarrow \infty$ , and in the opposite case where  $r = 1$  (all the phases are equal to zero, this a ‘‘completely resonant case’’),  $H_l$  is constant with  $T$ . This hope is made quantitative below, and the precise bound (5.10) is the final result of this subsection.

In order to simplify the presentation, we will adopt the convention (5.4). We also need to introduce some notations.

Considering  $H_l$  as a function of the  $(l+1)$ -tuple  $(\omega_1, \dots, \omega_l, \omega_{l+1})$  (with  $\omega_{l+1} := 0$ ), we see from formula (5.5) that all the two-by-two differences  $\omega_k - \omega_j$

$(k, j = 1, \dots, (l+1))$  are involved in the denominators. On the other hand,  $H_l$  is clearly a smooth function of the  $\omega_i$ 's. This is easily seen from the very definition of  $H_l$ . Hence for a given  $(l+1)$ -tuple  $(\omega_1, \dots, \omega_l, \omega_{l+1})$ , it is natural to group equal  $\omega_i$ 's, as follows: using the symmetry of  $H_l$  in  $(\omega_1, \dots, \omega_l)$ , we can always assume (up to re-indexing the  $\omega_i$ 's) that there exist integer numbers,

$$\begin{aligned} r \geq 1, a_1 \geq 1, \dots, a_r \geq 1, \\ \text{such that } a_1 + \dots + a_r = l + 1, \end{aligned} \quad (5.6)$$

and the following holds,

$$\begin{aligned} \Omega_1 &:= \omega_1 = \omega_2 = \dots = \omega_{a_1} \\ \Omega_2 &:= \omega_{a_1+1} = \omega_{a_1+2} = \dots = \omega_{a_1+a_2} \\ &\vdots \\ \Omega_{r-1} &:= \omega_{a_1+\dots+a_{r-2}+1} = \omega_{a_1+\dots+a_{r-2}+2} = \dots = \omega_{a_1+\dots+a_{r-1}} \\ \Omega_r &:= \omega_{a_1+\dots+a_{r-1}+1} = \dots = \omega_{a_1+\dots+a_r} = 0. \end{aligned} \quad (5.7)$$

This serves as a definition for the quantities  $\Omega_1, \dots, \Omega_r$  naturally associated with any given  $(l+1)$ -tuple  $(\omega_1, \dots, \omega_l, \omega_{l+1})$ . Using these notations, we implicitly assume that different  $\Omega_i$ 's have different values i.e.,

$$\Omega_i \neq \Omega_j, \quad \forall i \neq j. \quad (5.8)$$

Obviously the number  $r$  represents the number of different  $\omega_i$ 's in  $H_l$  as mentioned above. With these notations, we easily prove the,

**Lemma 2** *Under the notations and conventions (5.4), (5.6), (5.7), and (5.8), the following bound holds on the quantity  $H_l$ ,*

$$|H_l(\omega_1, \dots, \omega_l)| \leq \frac{C(t, l)}{\mathcal{T}^{r-1}} \sum_{s=1}^r \frac{1}{\prod_{\substack{s'=1 \\ s' \neq s}}^r |\Omega_s - \Omega_{s'}|}. \quad (5.9)$$

**Proof of Lemma 2**

Using the convention (5.7), we write,

$$\begin{aligned} |H_l|(\omega_1, \dots, \omega_l) &= |H_l|(\underbrace{\Omega_1, \dots, \Omega_1}_{a_1 \text{ terms}}, \dots, \underbrace{\Omega_{r-1}, \dots, \Omega_{r-1}}_{a_{r-1} \text{ terms}}, \underbrace{0, \dots, 0}_{a_r \text{ terms}}) \\ &= |H_l|(\underbrace{\Omega_1, \dots, \Omega_1}_{a_1-1 \text{ terms}}, \dots, \underbrace{\Omega_{r-1}, \dots, \Omega_{r-1}}_{a_{r-1}-1 \text{ terms}}, \underbrace{0, \dots, 0}_{a_r \text{ terms}}, \Omega_1, \Omega_2, \dots, \Omega_{r-1}), \end{aligned}$$

where we used the symmetry of  $H_l$  in  $(\omega_1, \dots, \omega_l)$ . Now, using the well-known fact,

$$\int_{s_1=0}^t \dots \int_{s_n=0}^{t-s_1-\dots-s_{n-1}} 1 ds_1 \dots ds_n = \frac{t^n}{n!},$$



with the value  $n = (a_1 - 1) + (a_2 - 1) + \dots + (a_{r-1} - 1) + (a_r - 1) = l + 1 - r$ , we obtain,

$$\begin{aligned}
& |H_l(\omega_1, \dots, \omega_l)| \\
& \leq \frac{|t|^{(a_1-1)+(a_2-1)+\dots+(a_{r-1}-1)+(a_r-1)}}{[(a_1 - 1) + (a_2 - 1) + \dots + (a_{r-1} - 1) + (a_r - 1)]!} \\
& \times \sup_{t \in \mathbb{R}} \left| \int_{s_1=0}^t \dots \int_{s_{r-1}=0}^{t-s_1-\dots-s_{r-2}} \exp(i\mathcal{T}[s_1\Omega_1 + \dots + s_{r-1}\Omega_{r-1}]) \right| \\
& \leq \frac{|t|^{l+1-r}}{(l+1-r)!} \frac{1}{\mathcal{T}^{r-1}} \sum_{s=1}^r \frac{1}{\prod_{\substack{s'=1 \\ s' \neq s}}^r |\Omega_s - \Omega_{s'}|} \tag{5.10}
\end{aligned}$$

and the last line comes from the use of the explicit formula (5.5). The Lemma is proved.  $\square$

### 5.3 Part II of the proof: Asymptotic behaviour of $\mathcal{Q}_{l,l'}(t)$

#### 5.3.1 The splitting of $\mathcal{Q}_{l,l'}(t)$

According to the splitting of  $\mathbb{Z}^{d(l+l'+1)}$  into a “resonant” set (5.3) and its complementary set, we define the resonant part of  $\mathcal{Q}_{l,l'}(t)$  as,

$$\begin{aligned}
\mathcal{Q}_{l,l'}^{\text{res}}(t) &= \frac{1}{L^{d+(l+l')(d-2)}} \sum_{\text{res}} \frac{t^{l+l'}}{l! l'!} \mathcal{V}_l\left(\frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L}\right) \tag{5.11} \\
& \times \mathcal{V}_l^*\left(\frac{p}{L}, \frac{j_1}{L}, \dots, \frac{j_{l'-1}}{L}, \frac{m}{L}\right) \rho^0\left(\frac{m}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right),
\end{aligned}$$

where the symbol  $\sum_{\text{res}} \dots$  means the sum over the “resonant” set (5.3). The term  $\mathcal{Q}_{l,l'}^{\text{res}}(t)$  is exactly the contribution of the resonant set (5.3) to  $\mathcal{Q}_{l,l'}(t)$ . Also, we may define the non-resonant term  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$  as,

$$\begin{aligned}
\mathcal{Q}_{l,l'}^{\text{nr}}(t) &= \frac{1}{L^{d+(l+l')(d-2)}} \sum_{\text{nr}} \exp(i\mathcal{T}t[n^2 - p^2]) \tag{5.12} \\
& \times H_l(m^2 - n^2, \dots, m^2 - k_{l-1}^2) H_{l'}(p^2 - m^2, \dots, j_{l'-1}^2 - m^2) \\
& \times \mathcal{V}_l\left(\frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L}\right) \mathcal{V}_l^*\left(\frac{p}{L}, \frac{j_1}{L}, \dots, \frac{j_{l'-1}}{L}, \frac{m}{L}\right) \rho^0\left(\frac{m}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right),
\end{aligned}$$

where the sum  $\sum_{\text{nr}} \dots$  is extended to the non-resonant set defined as the complementary set to the resonant set (5.3).

#### 5.3.2 The convergence of the non-resonant term $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$ towards zero

In this section, we prove the following,

**Theorem 3** *The non-resonant term is estimated by,*

$$\left| \mathcal{Q}_{l,l'}^{\text{nr}}(t) \right| \leq C(\varepsilon, t, l, l', \Phi) \frac{L^\varepsilon \log L}{\mathcal{T}}, \quad (5.13)$$

for some constant  $C(\varepsilon, t, l, l', \Phi)$  depending in particular on  $\varepsilon > 0$ . The value  $\varepsilon = 0$  is allowed in dimensions  $d \geq 5$ . Hence, as  $L$  and  $\mathcal{T}$  go to infinity in the regime (2.7) we have,

$$\mathcal{Q}_{l,l'}^{\text{nr}}(t) \rightarrow 0. \quad (5.14)$$

**Remark 10** Under the assumption **(A')**, the only uniform estimate we are able to prove on  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$  is actually of the form,

$$\left| \mathcal{Q}_{l,l'}^{\text{nr}}(t) \right| \leq C(\varepsilon, t, \Phi)^{l+l'} (l! l')^{\frac{d}{2}-2} \frac{L^\varepsilon \log L}{\mathcal{T}}. \quad (5.15)$$

For dimensions  $d \geq 5$ , the presence of factorial terms on the right-hand-side of (5.15) is the very reason for the fact that we are only able, in this paper, to prove the *term-by-term* convergence of the series,  $\langle \rho_I(t), \Phi \rangle = \sum_{l,l'} (-i\Lambda)^l (+i\Lambda)^{l'} \mathcal{Q}_{l,l'}(t)$ , and not the stronger convergence of the full series. The above estimate may be useful in dimension 3. Since we are not able to prove **(A')** in this case yet, we do not give the proof of the precise estimate (5.15) and simply prove the weaker bound (5.13) for the sake of simplicity.  $\square$

### Proof of Theorem 3

The proof of (5.13) is decomposed into several steps.

*First step: The splitting of  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$*

In view of the bound (5.9) obtained on  $H_l$  above, we need to split further the sum over the integers  $(m, n, p, k_1, \dots, k_{l-1}, j_1, \dots, j_{l'-1})$  which defines the term  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$ . Namely for a given value of  $(m, n, p, k_1, \dots)$ , we may introduce the vectors,

$$(\omega_1, \dots, \omega_l, \omega_{l+1}) := (m^2 - n^2, m^2 - k_1^2, \dots, m^2 - k_{l-1}^2, 0), \quad (5.16)$$

together with,

$$(\omega'_1, \dots, \omega'_l, \omega'_{l+1}) := (m^2 - p^2, m^2 - j_1^2, \dots, m^2 - j_{l'-1}^2, 0). \quad (5.17)$$

From its definition we know that  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$  is defined as a sum over the integers  $m, n, p, k_1, \dots$ , such that,

$$(\omega_1, \dots, \omega_{l+1}, \omega'_1, \dots, \omega'_{l'+1}) \neq (0, \dots, 0). \quad (5.18)$$

Now, following the discussion made in bounding  $H_l$  above, we split the sum over  $(m, n, p, k_1, \dots)$  as follows.

For a given value of  $(m, n, p, k_1, \dots)$ , let  $r$  be the number of different components in the vector,

$$(\omega_1, \dots, \omega_l, \omega_{l+1}),$$

and  $r'$  be the number of different components in the vector,

$$(\omega'_1, \dots, \omega'_l, \omega'_{l'+1}).$$

From the definition of the non-resonant term  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$ , we readily have,

$$1 \leq r \leq l+1, \quad 1 \leq r' \leq l'+1, \quad 2 < r+r' \leq l+l'+2. \quad (5.19)$$

Now, up to renaming the variables, we may assume, using the symmetry of  $H_l$  upon its arguments, that we can find integers,

$$a_1 \geq 1, \dots, a_r \geq 1, \quad \text{such that,} \quad a_1 + \dots + a_r = l+1, \quad (5.20)$$

and,

$$b_1 \geq 1, \dots, b_{r'} \geq 1, \quad \text{such that,} \quad b_1 + \dots + b_{r'} = l'+1, \quad (5.21)$$

and the following relations are satisfied,

$$\begin{aligned} \Omega_1 &:= \omega_1 = \omega_2 = \dots = \omega_{a_1} \\ \Omega_2 &:= \omega_{a_1+1} = \omega_{a_1+2} = \dots = \omega_{a_1+a_2} \\ &\vdots \\ \Omega_{r-1} &:= \omega_{a_1+a_2+\dots+a_{r-2}+1} = \omega_{a_1+a_2+\dots+a_{r-2}+2} = \dots = \omega_{a_1+a_2+\dots+a_{r-1}} \\ \Omega_r &:= \omega_{a_1+\dots+a_{r-1}+1} = \dots = \omega_{a_1+\dots+a_r} = 0, \end{aligned} \quad (5.22)$$

and,

$$\begin{aligned} \Omega'_1 &:= \omega'_1 = \omega'_2 = \dots = \omega'_{b_1} \\ \Omega'_2 &:= \omega'_{b_1+1} = \omega'_{b_1+2} = \dots = \omega'_{b_1+b_2} \\ &\vdots \\ \Omega'_{r'-1} &:= \omega'_{b_1+b_2+\dots+b_{r'-2}+1} = \omega'_{b_1+b_2+\dots+b_{r'-2}+2} = \dots = \omega'_{b_1+b_2+\dots+b_{r'-1}} \\ \Omega'_{r'} &:= \omega'_{b_1+\dots+b_{r'-1}+1} = \dots = \omega'_{b_1+\dots+b_{r'}} = 0. \end{aligned} \quad (5.23)$$

This serves as a definition for the integers  $(\Omega_1, \dots, \Omega_r)$  together with  $(\Omega'_1, \dots, \Omega'_{r'})$ , which are conventionnaly assumed all different (i.e.  $\Omega_i \neq \Omega_j, \forall i \neq j$ , and  $\Omega'_i \neq \Omega'_j, \forall i \neq j$ ).

In this perspective, the non-resonant term  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$  can be decomposed as a sum over all possible values of  $r, r', \underline{a} := (a_1, \dots, a_r), \underline{b} := (b_1, \dots, b_{r'})$  such that (5.19), (5.20), (5.21) are fulfilled, of a sum of all the contributions stemming from integers  $(m, n, p, k_1, \dots)$  satisfying (5.16), (5.17), together with (5.22) and (5.23). We thus define, for any such values of  $r, r', \underline{a} = (a_1, \dots, a_r), \underline{b} = (b_1, \dots, b_{r'})$ , the quantity,

$$\begin{aligned} \mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t) &:= \frac{1}{L^{d+(l+l')(d-2)}} \sum_{\text{nr}^*} \exp(i\mathcal{T}t[n^2 - p^2]) \\ &\times H_l(m^2 - n^2, \dots, m^2 - k_{l-1}^2) H_{l'}(p^2 - m^2, \dots, j_{l'-1}^2 - m^2) \\ &\times \mathcal{V}_l\left(\frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L}\right) \mathcal{V}_{l'}^*\left(\frac{p}{L}, \frac{j_1}{L}, \dots, \frac{j_{l'-1}}{L}, \frac{m}{L}\right) \rho^0\left(\frac{m}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right), \end{aligned} \quad (5.24)$$

where the symbol  $\sum_{\text{nr}^*} \dots$  denotes the sum over all possible integers  $(m, n, p, k_1, \dots, k_{l-1}, j_1, \dots, j_{l'-1})$  such that the above mentioned constraints are satisfied. Under these notations, we have the following splitting of  $\mathcal{Q}_{l,l'}^{\text{nr}}(t)$ ,

$$\mathcal{Q}_{l,l'}^{\text{nr}}(t) = \sum_{r,r',a_1,\dots,a_r,b_1,\dots,b_{r'}} \mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t), \quad (5.25)$$

where the sum is extended over all possible values of  $(r, r', a_1, \dots, a_r, b_1, \dots, b_{r'})$  such that (5.19), (5.20) and (5.21) are satisfied.

*Second step: a bound on  $\mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t)$*

According to the splitting (5.25) we now take some given value of the parameters  $r, r', (a_1, \dots, a_r), (b_1, \dots, b_{r'})$  as in (5.19), (5.20), (5.21), and we turn to bounding the contribution  $\mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t)$ . We actually prove that it is bounded like,

$$|\mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t)| \leq C(\varepsilon, t, l, l', \Phi) \frac{L^\varepsilon \log L}{\mathcal{T}}, \quad (5.26)$$

for some constant  $C(\varepsilon, t, l, l', \Phi)$  as in (5.13). Clearly, proving (5.26) is enough to establish (5.13).

In order to establish (5.26), we bound separately in (5.24) the factors  $H_l(\dots)$ ,  $H_{l'}(\dots)$  on the one hand, and  $\mathcal{V}_l(\dots)$ ,  $\mathcal{V}_{l'}^*(\dots)\rho^0(\dots)\Phi(\dots)$  on the other hand.

Firstly, on the set defining  $\mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t)$ , and with the convention (5.16), (5.17), we can use the upper bound on  $H_l$  obtained in (5.9), and thus write in (5.24),

$$|H_l(m^2 - n^2, \dots, m^2 - k_{l-1}^2)| \leq \frac{C(t, l)}{\mathcal{T}^{r-1}} \sum_{\alpha=1}^r \frac{1}{\prod_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^r |\Omega_{\alpha'} - \Omega_\alpha|}, \quad (5.27)$$

together with,

$$|H_{l'}(p^2 - m^2, \dots, j_{l'-1}^2 - m^2)| \leq \frac{C(t, l')}{\mathcal{T}^{r'-1}} \sum_{\beta=1}^{r'} \frac{1}{\prod_{\substack{\beta'=1 \\ \beta' \neq \beta}}^{r'} |\Omega'_{\beta'} - \Omega'_\beta|}. \quad (5.28)$$

Recall that all the two-by-two differences  $|\Omega_\alpha - \Omega_{\alpha'}|$  and  $|\Omega_\beta - \Omega_{\beta'}|$  are conventionally non-vanishing (hence they are  $\geq 1$ ).

Secondly, we may use the bound (4.6) to bound the factors involving  $\mathcal{V}_l$ . Also, we may use the decay assumption on  $\rho^0$  under the form  $|\rho^0(\mathbf{n})| \leq C\langle \mathbf{n}^2 \rangle^{-M}$  for some large value  $M$  to be chosen later, together with  $|\Phi(\dots)| \leq C(\Phi)$ . Hence we

may bound in (5.24),

$$\begin{aligned} & \left| \mathcal{V}_l\left(\frac{n}{L}, \dots, \frac{m}{L}\right) \mathcal{V}_{l'}^*\left(\frac{p}{L}, \dots, \frac{m}{L}\right) \rho^0\left(\frac{m}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right) \right| \\ & \leq C(l, l', \Phi) \left\langle \frac{n^2 - k_1^2}{L^2} \right\rangle^{-M} \dots \left\langle \frac{k_{l-1}^2 - m^2}{L^2} \right\rangle^{-M} \\ & \quad \times \left\langle \frac{p^2 - j_1^2}{L^2} \right\rangle^{-M} \dots \left\langle \frac{j_{l-1}^2 - m^2}{L^2} \right\rangle^{-M} \left\langle \frac{m^2}{L^2} \right\rangle^{-M}. \end{aligned}$$

Using the constraints (5.22) and (5.23) allows to rewrite this upper-bound in terms of the variables  $\Omega_i$  ( $i = 1, \dots, r$ ),  $\Omega'_i$  ( $i = 1, \dots, r'$ ), and  $m$ , giving,

$$\begin{aligned} & \left| \mathcal{V}_l\left(\frac{n}{L}, \dots, \frac{m}{L}\right) \mathcal{V}_{l'}^*\left(\frac{p}{L}, \dots, \frac{m}{L}\right) \rho^0\left(\frac{m}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right) \right| \\ & \leq C(l, l', \Phi) \left\langle \frac{\Omega_1 - \Omega_2}{L^2} \right\rangle^{-M} \dots \left\langle \frac{\Omega_{r-2} - \Omega_{r-1}}{L^2} \right\rangle^{-M} \left\langle \frac{\Omega_{r-1}}{L^2} \right\rangle^{-M} \\ & \quad \times \left\langle \frac{\Omega'_1 - \Omega'_2}{L^2} \right\rangle^{-M} \dots \left\langle \frac{\Omega'_{r'-2} - \Omega'_{r'-1}}{L^2} \right\rangle^{-M} \left\langle \frac{\Omega'_{r'-1}}{L^2} \right\rangle^{-M} \left\langle \frac{m^2}{L^2} \right\rangle^{-M} \\ & \leq C(l, l') \left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{-M} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{-M} \right] \left\langle \frac{m^2}{L^2} \right\rangle^{-M}. \end{aligned} \quad (5.29)$$

Combining (5.27), (5.28) and (5.29) together gives in (5.24),

$$\begin{aligned} \left| \mathcal{Q}_{l, l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t) \right| & \leq \frac{C(t, l, l', \Phi)}{\mathcal{T}^{r+r'-2}} \frac{1}{L^{d+(l+l')(d-2)}} \\ & \times \sum_{\substack{m, \Omega_1, \dots, \Omega_{r-1}, \\ \Omega'_1, \dots, \Omega'_{r'-1}}} \left[ \sum_{\alpha=1}^r \frac{1}{\prod_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^r |\Omega_{\alpha'} - \Omega_{\alpha}|} \right] \left[ \sum_{\beta=1}^{r'} \frac{1}{\prod_{\substack{\beta'=1 \\ \beta' \neq \beta}}^{r'} |\Omega'_{\beta'} - \Omega'_{\beta}|} \right] \\ & \times \left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{-M} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{-M} \right] \left\langle \frac{m^2}{L^2} \right\rangle^{-M} \times \#_{m, \Omega, \Omega'}, \end{aligned} \quad (5.30)$$

up to defining,

$$\begin{aligned} \#_{m, \Omega, \Omega'} & := \#\{(m, k_0, \dots, k_{l-1}, j_0, \dots, j_{l'-1}) \\ & \text{s. t. (5.16), (5.17), (5.22), (5.23) hold } \}, \end{aligned} \quad (5.31)$$

and the sum in (5.30) is now extended over all possible values of  $m \in \mathbb{Z}^d$ ,  $\Omega$ 's and  $\Omega'$ 's in  $\mathbb{Z}$  such that the differences  $|\Omega_{\alpha} - \Omega_{\alpha'}|$  and  $|\Omega'_{\beta} - \Omega'_{\beta'}|$  do not vanish, a convention we keep throughout the remainder part of the present proof. This bound is analogous to the bound (3.2) of the model computation in section 3.

Thirdly, and analogously to the procedure of section 3, we may use the bound (2.29) to estimate the cardinality  $\#_{m, \Omega, \Omega'}$  above as (compare with (3.3)),

$$\begin{aligned} & \#_{m, \Omega, \Omega'} \\ & \leq C(\varepsilon) (m^2 - \Omega_1)^{\left(\frac{d}{2}-1+\varepsilon\right)a_1} \dots (m^2 - \Omega_{r-1})^{\left(\frac{d}{2}-1+\varepsilon\right)a_{r-1}} (m^2)^{\left(\frac{d}{2}-1+\varepsilon\right)(a_r-1)} \\ & \quad (m^2 - \Omega'_1)^{\left(\frac{d}{2}-1+\varepsilon\right)b_1} \dots (m^2 - \Omega'_{r'-1})^{\left(\frac{d}{2}-1+\varepsilon\right)b_{r'-1}} (m^2)^{\left(\frac{d}{2}-1+\varepsilon\right)(b_{r'}-1)}. \end{aligned}$$

Normalizing the right-hand-side by the correct power of  $L$  for future convenience, and separating the dependence upon the various variables gives,

$$\begin{aligned} \#_{m,\Omega,\Omega'} &\leq C(\varepsilon, l, l') [L^2]^{\left(\frac{d}{2}-1+\varepsilon\right)(a_1+\dots+a_r+b_1+\dots+b_{r'}-2)} \\ &\left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{\left(\frac{d}{2}-1+\varepsilon\right)a_i} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{\left(\frac{d}{2}-1+\varepsilon\right)b_i} \right] \\ &\left\langle \frac{m^2}{L^2} \right\rangle^{\left(\frac{d}{2}-1+\varepsilon\right)(a_1+\dots+a_r+b_1+\dots+b_{r'}-2)}, \end{aligned}$$

and, using (5.20), (5.21) to observe that  $a_1 + \dots + a_r + b_1 + \dots + b_{r'} - 2 = l + l'$ , together with  $a_i \leq l$  and  $b_i \leq l'$  for all  $i$ , we get,

$$\begin{aligned} \#_{m,\Omega,\Omega'} &\leq C(\varepsilon, l, l') L^{(d-2+\varepsilon)(l+l')} \tag{5.32} \\ &\left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{\left(\frac{d}{2}-1+\varepsilon\right)l} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{\left(\frac{d}{2}-1+\varepsilon\right)l'} \right] \left\langle \frac{m^2}{L^2} \right\rangle^{\left(\frac{d}{2}-1+\varepsilon\right)(l+l')}. \end{aligned}$$

Fourthly, there remains to insert estimate (5.32) on the cardinality  $\#_{m,\Omega,\Omega'}$  in (5.30). This gives,

$$\begin{aligned} \left| \mathcal{Q}_{l,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t) \right| &\leq \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2} L^d} \tag{5.33} \\ &\times \sum_{\substack{m, \Omega_1, \dots, \Omega_{r-1}, \\ \Omega'_1, \dots, \Omega'_{r'-1}}} \left[ \sum_{\alpha=1}^r \frac{1}{\prod_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^r |\Omega_{\alpha'} - \Omega_\alpha|} \right] \left[ \sum_{\beta} \frac{1}{\prod_{\substack{\beta'=1 \\ \beta' \neq \beta}}^{r'} |\Omega'_{\beta'} - \Omega'_\beta|} \right] \\ &\times \left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{-M+l} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{-M+l'} \right] \left\langle \frac{m^2}{L^2} \right\rangle^{-M+l+l'}. \end{aligned}$$

There only remains now to estimate the reference sum on the right-hand-side of (5.33). From now on, we assume that the exponent  $M$  is chosen so large that  $M - l \geq 2$ ,  $M - l' \geq 2$ , and  $M - l - l' \geq d + 2$ .

*Third step: estimating (5.33) for small values of the denominators  $|\Omega_\alpha - \Omega_{\alpha'}|$ ,  $|\Omega'_\beta - \Omega'_{\beta'}|$*

The right-hand-side of (5.33) is estimated upon separating, for each pair  $(\alpha, \alpha')$  and  $(\beta, \beta')$ , the cases  $|\Omega_\alpha - \Omega_{\alpha'}| \leq L^2$  and  $|\Omega_\alpha - \Omega_{\alpha'}| \geq L^2$ , and similarly for  $|\Omega'_\beta - \Omega'_{\beta'}|$ . This gives rise to  $2^{l+l'}$  different cases. The present step is devoted to the study of the case where *all* the above mentioned differences are  $\leq L^2$ . The next step studies the opposite extreme case where all these differences are  $\geq L^2$ . All the other intermediate cases are easily treated upon combining accordingly the different techniques we propose here.

In the present case, the key lies in *first* majorizing all the decaying factors  $\langle \Omega_i/L^2 \rangle^{-M+l}$  and  $\langle \Omega'_i/L^2 \rangle^{-M+l'}$  by one, *secondly* using that  $\sum_{\gamma=1}^{L^2} \gamma^{-1} \leq C \log L$ , for  $\gamma = |\Omega_\alpha - \Omega_{\alpha'}|$ , and *thirdly* using that  $L^{-d} \sum_m \langle m^2/L^2 \rangle^{-M+l+l'} \leq C$ , see (2.31). Indeed,

$$\begin{aligned}
& \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2} L^d} \\
& \sum_{\substack{m, \Omega_1, \dots, \Omega_{r-1}, \\ \Omega'_1, \dots, \Omega'_{r'-1}}} \left[ \sum_{\alpha=1}^r \prod_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^r \frac{\mathbf{1}[|\Omega_\alpha - \Omega_{\alpha'}| \leq L^2]}{|\Omega_{\alpha'} - \Omega_\alpha|} \right] \langle \frac{m^2}{L^2} \rangle^{-M+l+l'} \\
& \times \left[ \sum_{\beta=1}^{r'} \prod_{\substack{\beta'=1 \\ \beta' \neq \beta}}^{r'} \frac{\mathbf{1}[|\Omega'_\beta - \Omega'_{\beta'}| \leq L^2]}{|\Omega'_{\beta'} - \Omega'_\beta|} \right] \left[ \prod_{i=1}^{r-1} \langle \frac{\Omega_i}{L^2} \rangle^{-M+l} \right] \left[ \prod_{i=1}^{r'-1} \langle \frac{\Omega'_i}{L^2} \rangle^{-M+l'} \right] \\
& \leq \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2}} \left[ \sum_{\Omega_1, \dots, \Omega_{r-1}} \sum_{\alpha=1}^r \prod_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^r \frac{\mathbf{1}[|\Omega_\alpha - \Omega_{\alpha'}| \leq L^2]}{|\Omega_{\alpha'} - \Omega_\alpha|} \right] \\
& \left[ \sum_{\Omega'_1, \dots, \Omega'_{r'-1}} \sum_{\beta=1}^{r'} \prod_{\substack{\beta'=1 \\ \beta' \neq \beta}}^{r'} \frac{\mathbf{1}[|\Omega'_\beta - \Omega'_{\beta'}| \leq L^2]}{|\Omega'_{\beta'} - \Omega'_\beta|} \right] \left[ \frac{1}{L^d} \sum_m \langle \frac{m^2}{L^2} \rangle^{-M+l+l'} \right] \\
& \leq \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2}} [\log L]^{r-1} [\log L]^{r'-1} \\
& = C(\varepsilon, t, l, l', \Phi) \left( \frac{L^\varepsilon \log L}{\mathcal{T}} \right)^{r+r'-2}. \tag{5.34}
\end{aligned}$$

As a conclusion, (5.34) establishes that the contribution to  $\mathcal{Q}_{i,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t)$  due to  $\Omega$ 's and  $\Omega'$ 's such that the corresponding two-by-two differences are all  $\leq L^2$  satisfies indeed the estimate (5.13) of Theorem 3 in the regime (2.7) (indeed we know that  $r + r' > 2$ , from (5.19)).

*Fourth step: estimating (5.33) for large values of the denominators  $|\Omega_\alpha - \Omega_{\alpha'}|$ ,  $|\Omega'_\beta - \Omega'_{\beta'}|$*

As explained in the previous step, we now turn to estimating the contribution to  $\mathcal{Q}_{i,l'}^{\text{nr}}[r, r', \underline{a}, \underline{b}](t)$  due to  $\Omega$ 's and  $\Omega'$ 's such that the corresponding two-by-two differences are all  $\geq L^2$ . Now the idea lies in *first* majorizing all the factors  $1/|\Omega_\alpha - \Omega_{\alpha'}|$  by  $1/L^2$  and the same for the primed variables, and *secondly* majorizing the re-

maining sum over  $m$ ,  $\Omega$ 's, and  $\Omega'$ 's as a simple Riemann sum, using (2.31). Indeed,

$$\begin{aligned}
& \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2} L^d} \\
& \sum_{\substack{m, \Omega_1, \dots, \Omega_{r-1}, \\ \Omega'_1, \dots, \Omega'_{r'-1}}} \left[ \sum_{\alpha=1}^r \prod_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^r \frac{\mathbf{1}[|\Omega_\alpha - \Omega_{\alpha'}| \geq L^2]}{|\Omega_{\alpha'} - \Omega_\alpha|} \right] \left\langle \frac{m^2}{L^2} \right\rangle^{-M+l+l'} \\
& \times \left[ \sum_{\beta=1}^r \prod_{\substack{\beta'=1 \\ \beta' \neq \beta}}^{r'} \frac{\mathbf{1}[|\Omega'_\beta - \Omega'_{\beta'}| \geq L^2]}{|\Omega'_{\beta'} - \Omega'_\beta|} \right] \left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{-M+l} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{-M+l'} \right] \\
& \leq \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2} L^{d+2(r-1)+2(r'-1)}} \\
& \times \sum_{\substack{m, \Omega_1, \dots, \Omega_{r-1}, \\ \Omega'_1, \dots, \Omega'_{r'-1}}} \left[ \prod_{i=1}^{r-1} \left\langle \frac{\Omega_i}{L^2} \right\rangle^{-M+l} \right] \left[ \prod_{i=1}^{r'-1} \left\langle \frac{\Omega'_i}{L^2} \right\rangle^{-M+l'} \right] \left\langle \frac{m^2}{L^2} \right\rangle^{-M+l+l'} \\
& \leq \frac{C(\varepsilon, t, l, l', \Phi) L^\varepsilon}{\mathcal{T}^{r+r'-2}}. \tag{5.35}
\end{aligned}$$

As a conclusion, (5.35) establishes that the contribution to  $\mathcal{Q}_{i,l'}^{\text{rr}}[r, r', \underline{a}, \underline{b}](t)$  due to  $\Omega$ 's and  $\Omega'$ 's such that the corresponding two-by-two differences are all  $\geq L^2$  satisfies indeed the estimate (5.13) of Theorem 3 (it satisfies actually a stronger estimate).

*Last step: conclusion*

The third and fourth steps of the present proof are enough to prove that the full term  $\mathcal{Q}_{i,l'}^{\text{rr}}[r, r', \underline{a}, \underline{b}](t)$  satisfies indeed (5.13). This is done upon combining the techniques used in these steps to treat the general contribution when some differences  $|\Omega_\alpha - \Omega_{\alpha'}|$  are  $\leq L^2$  and some are  $\geq L^2$  (and the same for primed variables). Hence the non-resonant term  $\mathcal{Q}_{i,l'}^{\text{rr}}(t)$  itself satisfies (5.13) and Theorem 3 is proved.  $\square$

### 5.3.3 The limit of $\mathcal{Q}_{i,l'}(t)$

From the above subsection we have the equivalence,

$$\mathcal{Q}_{i,l'}(t) \sim \mathcal{Q}_{i,l'}^{\text{res}}(t),$$

as  $L$  and  $\mathcal{T}$  go to infinity in the regime (2.7) under consideration. It remains to compute the actual limit of the resonant term  $\mathcal{Q}_{i,l'}^{\text{res}}(t)$ , where, as we already observed (see (5.11)),

$$\mathcal{Q}_{i,l'}^{\text{res}}(t) = \frac{1}{L^{d+(d-2)(l+l')}} \sum_{\text{res}} \frac{t^{l+l'}}{l! l'!} \mathcal{V}_l \left( \frac{n}{L}, \frac{k_1}{L}, \dots, \frac{k_{l-1}}{L}, \frac{m}{L} \right)$$



$$\times \mathcal{V}_l^* \left( \frac{p}{L}, \frac{j_1}{L}, \dots, \frac{j_{l'-1}}{L}, \frac{m}{L} \right) \rho^0 \left( \frac{m}{L} \right) \Phi \left( \frac{n}{L}, \frac{p}{L} \right),$$

and the symbol  $\sum_{\text{res}} \dots$  denotes a sum over the resonant set (5.3) as before. Now, it is an easy consequence of the Theorem 2 (Riemann sums with quadratic constraints) that this term actually converges towards  $\mathcal{Q}_{l,l'}^\infty(t)$  as defined in Proposition 2, equation (5.1). This concludes the proof of Proposition 2, hence the proof of Theorem 1 upon using Theorem 2.

## 6 Proof of Theorem 2: Riemann sums with quadratic constraints

In this section we prove Theorem 2 using assumption **(A)**.

Before proving Theorem 2, we first state the following Lemma, which is a consequence of the asymptotic formulae (2.22) and (2.23) proved in [CP]. Theorem 2 turns out to be an easy consequence of the present Lemma.

**Lemma 3** *Let  $\phi$  be as in Theorem 2, with a dimension  $d \geq 3$ , and assume **(A)** holds true. Consider the sum,*

$$J_{A,\delta}(\phi) := \frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \frac{1}{B^{(N+1)(\frac{d}{2}-1)}} \quad (6.1)$$

$$\times \sum_{(k_0, \dots, k_N) \in \mathbb{Z}^{(N+1)d}} \phi \left( \frac{k_0}{\sqrt{B}}, \dots, \frac{k_N}{\sqrt{B}} \right) \mathbf{1}[k_0^2 = \dots = k_N^2 = B].$$

Assume finally that  $0 < \delta < \delta_0(d)$  and moreover  $\delta < 3/4$  in dimension  $d = 3$ . Then, the following asymptotic holds true,

$$J_{A,\delta}(\phi) \xrightarrow{A \rightarrow \infty} \gamma_{N+1,d} \int_{\mathbb{S}^{(N+1)(d-1)}} \phi(\mathbf{k}_0, \dots, \mathbf{k}_N) d\sigma(\mathbf{k}_0) \dots d\sigma(\mathbf{k}_N). \quad (6.2)$$

**Remark 11** Here and throughout this Section we will use the following two notations. At first, for any  $A \in \mathbb{N}$ , we associate the cardinality,

$$\#_A := \#\{n \in \mathbb{Z}^d \text{ s.t. } n^2 = A\}. \quad (6.3)$$

Also, for a given  $A \in \mathbb{N}$  and a given solid angle  $\Omega \subset \mathbb{S}^{d-1}$ , we introduce the cardinality,

$$\#_{A,\Omega} := \#\{n \in \mathbb{Z}^d \text{ s.t. } n^2 = A \text{ and } \frac{n}{|n|} \in \Omega\}. \quad (6.4)$$

□

**Remark 12** Note that Lemma 3 gives a “localized” version of Theorem 2 in that it considers limits of the type  $I_N(\phi)$  as in Theorem 2 when the common value  $k_0^2 = \dots = k_N^2 = B$  fluctuates of an amount  $O(A^{1-\delta})$  around the fixed value  $A$ , whereas this value  $B$  can take any value between 0 and  $L^2$  in Theorem 2. □

### Proof of Lemma 3

The proof is given in several steps.

*First step: preliminary observations*

At first we observe from the well-known asymptotics (2.24) that assumption **(A)** readily transforms into,

$$\frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^l \xrightarrow{A \rightarrow \infty} \gamma_{l,d} \left( \frac{\Gamma(d/2)}{\Gamma(3/2)^d} \right)^l . \quad (6.5)$$

In particular, the right-hand-side of (6.5) is bounded, i.e.,

$$\frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^l \leq C(l) , \quad (6.6)$$

for some constant  $C(l)$ . Note that the assumption **(A')** even asserts  $C(l) = C^l$ .

The second observation lies in the fact that it is enough to prove the Lemma when  $\phi$  is of the form,

$$\phi(\mathbf{k}_0, \dots, \mathbf{k}_N) = \mathbf{1}(k_0 \in \Omega_0) \dots \mathbf{1}(\mathbf{k}_N \in \Omega_N) , \quad (6.7)$$

for some solid angles  $\Omega_0 \subset \mathbb{S}^{d-1}$ ,  $\dots$ ,  $\Omega_N \subset \mathbb{S}^{d-1}$ . Indeed, we have the following obvious bound,

$$\begin{aligned} |J_{A,\delta}| &\leq \|\phi\|_{L^\infty} \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \frac{1}{B^{(N+1)(\frac{d}{2}-1)}} (\#B)^{N+1} \\ &\leq C(N) \|\phi\|_{L^\infty} \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^{N+1} \\ &\leq C(N) \|\phi\|_{L^\infty} , \end{aligned}$$

where the second line comes from using the asymptotics (2.24), and the last line comes from assumption **(A)** under the form (6.5). On the more, it is clear from (6.2) that the sum  $J_{A,\delta}(\phi)$  only involves the dependence of  $\phi$  upon the angular variables  $\mathbf{k}_0/|\mathbf{k}_0|, \dots, \mathbf{k}_N/|\mathbf{k}_N|$ . Now, since linear combinations of functions of the form (6.7) is dense in the set of smooth functions  $\phi$  defined over  $\mathbb{S}^{(d-1)(N+1)}$ , our claim (6.7) is proved.

The third and last observation is the following. As a consequence of (2.22) and (2.23), we have for any  $\Omega \subset \mathbb{S}^{d-1}$  and any  $0 < \delta < 1$  ( $\delta < 3/4$  in dimension  $d = 3$ ),

$$\frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \frac{\#_{B,\Omega}}{\#_B} \xrightarrow{A \rightarrow \infty} d\sigma(\Omega) . \quad (6.8)$$

Now we claim that (6.8) implies the following asymptotics, valid for any power  $P \in \mathbb{N}^*$ ,

$$\frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left( \frac{\#_{B,\Omega}}{\#_B} \right)^P \rightarrow_{A \rightarrow \infty} (d\sigma(\Omega))^P. \quad (6.9)$$

Let us indeed prove (6.9) from (6.8). By an easy induction on  $P$ , (6.9) is proved once the following limit is established,

$$\frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left[ \frac{\#_{B,\Omega}}{\#_B} - d\sigma(\Omega) \right] \left( \frac{\#_{B,\Omega}}{\#_B} \right)^P \rightarrow_{A \rightarrow \infty} 0, \quad (6.10)$$

for any  $P \in \mathbb{N}^*$ . Now (6.10) is proved by Abel summation,

$$\begin{aligned} & \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left[ \frac{\#_{B,\Omega}}{\#_B} - d\sigma(\Omega) \right] \left( \frac{\#_{B,\Omega}}{\#_B} \right)^P \\ &= \sum_{B=A}^{A+A^{1-\delta}} \frac{1}{1+A^{1-\delta}} \left[ \sum_{C=A}^B \left( \frac{\#_{C,\Omega}}{\#_C} \right) - d\sigma(\Omega) \right] \left[ \left( \frac{\#_{B,\Omega}}{\#_B} \right)^P - \left( \frac{\#_{B+1,\Omega}}{\#_{B+1}} \right)^P \right] \\ &+ \frac{1}{1+A^{1-\delta}} \left[ \sum_{C=A}^{A+A^{1-\delta}} \left( \frac{\#_{B,\Omega}}{\#_B} \right) - d\sigma(\Omega) \right] \\ &\quad \times \left[ \left( \frac{\#_{A+A^{1-\delta},\Omega}}{\#_{A+A^{1-\delta}}} \right)^P - \left( \frac{\#_{A+A^{1-\delta}+1,\Omega}}{\#_{A+A^{1-\delta}+1}} \right)^P \right]. \end{aligned} \quad (6.11)$$

On the one hand, for any  $B$  between  $A$  and  $A+A^{1-\delta}$ , it is clear that,

$$\frac{1}{1+A^{1-\delta}} \sum_{C=A}^B \left[ \left( \frac{\#_{C,\Omega}}{\#_C} \right) - d\sigma(\Omega) \right] \rightarrow_{A \rightarrow \infty} 0.$$

Indeed, this is clear when  $B-A = o(A^{1-\delta})$  by mere boundedness of the summand, and this is a consequence of (2.22) and (2.23) when  $B-A \geq C A^{1-\delta}$  for some constant  $C$ . On the other hand, we may bound,

$$\frac{\#_{B,\Omega}}{\#_B} \leq 1,$$

trivially. These two observations are enough to prove that the right-hand-side of (6.11) goes to zero, hence (6.9) is proved.

*Second step: proving the Lemma when (6.7) holds*

In this case we write,

$$\begin{aligned} J_{A,\delta}(\phi) &= \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \frac{1}{B^{\left(\frac{d}{2}-1\right)(N+1)}} \#_{B,\Omega_0} \cdots \#_{B,\Omega_N} \\ &\sim_{A \rightarrow \infty} \left( \frac{\Gamma(3/2)^d}{\Gamma(d/2)} \right)^{N+1} \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \frac{\#_{B,\Omega_0}}{\#_B} \cdots \frac{\#_{B,\Omega_N}}{\#_B} \mathfrak{S}(B)^{N+1}, \end{aligned}$$

where (2.24) has been used. Now, we claim that the following difference vanishes asymptotically,

$$\begin{aligned} & \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left[ \frac{\#_{B,\Omega_0}}{\#_B} \dots \frac{\#_{B,\Omega_N}}{\#_B} - d\sigma(\Omega_0) \dots d\sigma(\Omega_N) \right] \mathfrak{S}(B)^{N+1} \\ & \xrightarrow{A \rightarrow \infty} 0. \end{aligned} \quad (6.12)$$

Assuming (6.12) holds true for the moment, we deduce,

$$\begin{aligned} & J_{A,\delta}(\phi) \\ & \sim_{A \rightarrow \infty} \left( \frac{\Gamma(3/2)^d}{\Gamma(d/2)} \right)^{N+1} d\sigma(\Omega_0) \dots d\sigma(\Omega_N) \times \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^{N+1} \\ & \sim_{A \rightarrow \infty} \gamma_{N+1,d} d\sigma(\Omega_0) \dots d\sigma(\Omega_N), \end{aligned}$$

thanks to assumption **(A)** under the form (6.5). Hence the Lemma is proved when  $\phi$  is of the form (6.7), and formula (6.2) thus holds for any  $\phi$  by density.

There remains to prove (6.12). To do so it is enough to prove,

$$\frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left[ \left( \frac{\#_{B,\Omega_0}}{\#_B} - d\sigma(\Omega_0) \right) \frac{\#_{B,\Omega_1}}{\#_B} \dots \frac{\#_{B,\Omega_N}}{\#_B} \right] \mathfrak{S}(B)^{N+1} \xrightarrow{A \rightarrow \infty} 0.$$

The above convergence is an easy consequence of the subsequent majorisations,

$$\begin{aligned} & \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left[ \left( \frac{\#_{B,\Omega_0}}{\#_B} - d\sigma(\Omega_0) \right) \frac{\#_{B,\Omega_1}}{\#_B} \dots \frac{\#_{B,\Omega_N}}{\#_B} \right] \mathfrak{S}(B)^{N+1} \\ & \leq \left[ \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left( \frac{\#_{B,\Omega_0}}{\#_B} - d\sigma(\Omega_0) \right)^{N+2} \right]^{\frac{1}{N+2}} \\ & \left[ \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left( \frac{\#_{B,\Omega_1}}{\#_B} \right)^{N+2} \right]^{\frac{1}{N+2}} \dots \left[ \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left( \frac{\#_{B,\Omega_N}}{\#_B} \right)^{N+2} \right]^{\frac{1}{N+2}} \\ & \quad \left[ \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^{(N+1)(N+2)} \right]^{\frac{1}{N+2}} \\ & \leq C(N) \left[ \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \left( \frac{\#_{B,\Omega_0}}{\#_B} - d\sigma(\Omega_0) \right)^{N+2} \right]^{\frac{1}{N+2}} \\ & \xrightarrow{A \rightarrow \infty} 0 \end{aligned}$$

where the first inequality comes from using Hölder's inequality, and the second comes from the bounds (6.6) and (6.9), together with the obvious bound  $\#_{B, \Omega_i} / \#_B \leq 1$  for any  $i$ . This ends the proof of (6.12).  $\square$

### Proof of Theorem 2

Upon the use of Lemma 3 above, the proof of Theorem 2 now reduces essentially to the use of certain Riemann sums in the variable  $A$  of Lemma 3.

#### First Step

First of all, we have the obvious a priori bound,

$$\begin{aligned}
& L^{-N(d-2)-d} \sum_{k_0, \dots, k_N} \phi(L^{-1}k_0, L^{-1}k_1, \dots, L^{-1}k_N) \mathbf{1}[k_0^2 = k_1^2 = \dots = k_N^2] \\
& \leq \| \langle \mathbf{k}_0 \rangle^M \phi \|_{L^\infty} L^{-N(d-2)-d} \sum_{k_0} [\#\{k \in \mathbb{Z}^d \text{ s.t. } k^2 = k_0^2\}]^N \langle \frac{k_0}{L} \rangle^{-M} \\
& \leq C(N) \| \langle \mathbf{k}_0 \rangle^M \phi \|_{L^\infty} L^{-N(d-2)-d} \sum_{k_0} |k_0|^{N(d-2)} \langle \frac{k_0}{L} \rangle^{-M} \\
& \leq C(N) \| \langle \mathbf{k}_0 \rangle^M \phi \|_{L^\infty} L^{-d} \sum_{k_0} \langle \frac{k_0}{L} \rangle^{-M+N(d-2)} \\
& \leq C(N, M) \| \langle \mathbf{k}_0 \rangle^M \phi \|_{L^\infty} ,
\end{aligned}$$

for some constant  $C(N, M)$ , and for any  $M > N(d-2) + 1$ . Indeed, the third line uses the asymptotics (2.24), and the last line uses (2.31). By an easy density argument, it is thus enough to prove the Theorem in the case where  $\phi$  is of the form,

$$\begin{aligned}
\phi(\mathbf{k}_0, \dots, \mathbf{k}_N) &= \mathbf{1}[|\mathbf{k}_0| \leq R] \mathbf{1} \left[ \frac{\mathbf{k}_0}{|\mathbf{k}_0|} \in \Omega_0 \right] \mathbf{1} \left[ \frac{\mathbf{k}_1}{|\mathbf{k}_1|} \in \Omega_1 \right] \dots \mathbf{1} \left[ \frac{\mathbf{k}_N}{|\mathbf{k}_N|} \in \Omega_N \right] \\
&\quad \times \mathbf{1}[k_0^2 = \dots = k_N^2] ,
\end{aligned} \tag{6.13}$$

for some  $R > 0$ , and some solid angles  $\Omega_0 \subset \mathbb{S}^{d-1}, \dots, \Omega_N \subset \mathbb{S}^{d-1}$ .

#### Second Step

Let  $\phi$  be of the form (6.13). In this case, the ‘‘Riemann sum’’  $I_L(\phi)$  takes the form,

$$I_L(\phi) = \frac{1}{L^{N(d-2)+d}} \sum_{A=0}^{RL^2} \#_{A, \Omega_0} \dots \#_{A, \Omega_N} , \tag{6.14}$$

and we wish to pass to the limit  $L \rightarrow \infty$  in (6.14). In order to do so, we choose a small increment,

$$h = L^{-\frac{1}{4}} , \tag{6.15}$$

and we mention that there is a good deal of latitude in this choice of  $h$ . We decompose the sum over  $A$  defining  $I_L(\phi)$  into small “slices” of size  $hL^2$  accordingly,

$$I_L(\phi) = \frac{1}{L^{N(d-2)+d}} \sum_{t=0}^{(R^2/h)-1} \sum_{A=thL^2}^{(t+1)hL^2-1} \#_{A,\Omega_0} \cdots \#_{A,\Omega_N}. \quad (6.16)$$

Note that we assume here for convenience that all bounds appearing in the above sums are integer numbers.

Now, we wish to apply Lemma 3 to each sum  $\sum_{A=thL^2}^{(t+1)hL^2-1} \cdots$  in (6.16). To this aim, we first need to put the “small” values of  $A$  apart, as follows: let  $\eta > 0$  be an arbitrary small cutoff parameter, we write,

$$\begin{aligned} I_L(\phi) &= \frac{1}{L^{N(d-2)+d}} \sum_{t=0}^{(\eta/h)} \sum_{A=thL^2}^{(t+1)hL^2} \#_{A,\Omega_0} \cdots \#_{A,\Omega_N} \\ &\quad + \frac{1}{L^{N(d-2)+d}} \sum_{t=(\eta/h)}^{(R^2/h)-1} \sum_{A=thL^2}^{(t+1)hL^2} \#_{A,\Omega_0} \cdots \#_{A,\Omega_N} \\ &=: I_L^1(\phi) + I_L^2(\phi). \end{aligned} \quad (6.17)$$

This is the desired splitting of  $I_L(\phi)$ . We now study  $I_L^1(\phi)$  and  $I_L^2(\phi)$  separately.

*Third step: study of  $I_L^1(\phi)$*

The term  $I_L^1(\phi)$  is easily upper-bounded,

$$\begin{aligned} |I_L^1(\phi)| &= \frac{1}{L^{N(d-2)+d}} \sum_{A=0}^{(\eta+h)L^2} \#_{A,\Omega_0} \cdots \#_{A,\Omega_N} \\ &\leq \frac{1}{L^{N(d-2)+d}} \sum_{A=0}^{(\eta+h)L^2} (\#_A)^{N+1} \\ &\leq \frac{C(N)}{L^{N(d-2)+d}} \sum_{A=0}^{(\eta+h)L^2} \mathfrak{G}(A)^{N+1} A^{(N+1)(\frac{d}{2}-1)} \\ &\leq \frac{C(N)}{L^2} \sum_{A=0}^{(\eta+h)L^2} \mathfrak{G}(A)^{N+1} (\eta+h)^{(N+1)(\frac{d}{2}-1)} \\ &\leq C(N)(\eta+h)^{(N+1)(\frac{d}{2}-1)+1}, \end{aligned} \quad (6.18)$$

where the third line uses (2.24), and the last line uses assumption **(A)** under the form (6.6).

*Fourth step: limiting behaviour of  $I_L^2(\phi)$*

To be able to apply Lemma 3, we first rewrite  $I_L^2(\phi)$  under the form,

$$I_L^2(\phi) = h \sum_{t=(\eta/h)}^{(R^2/h)-1} \left( \frac{1}{hL^2} \sum_{A=thL^2}^{(t+1)hL^2} \frac{\#_{A,\Omega_0} \cdots \#_{A,\Omega_N}}{A^{(N+1)(\frac{d}{2}-1)}} \left( \frac{A}{L^2} \right)^{(N+1)(\frac{d}{2}-1)} \right).$$

Firstly, assumption **(A)** together with the obvious estimate  $\#_{A,\Omega} \leq \#_A$  valid for any  $\Omega$  allow to establish the equivalence,

$$I_L^2(\phi) \underset{L \rightarrow \infty}{\sim} h \sum_{t=(\eta/h)}^{(R^2/h)-1} (th)^{(N+1)(\frac{d}{2}-1)} \left( \frac{1}{hL^2} \sum_{A=thL^2}^{(t+1)hL^2} \frac{\#_{A,\Omega_0} \cdots \#_{A,\Omega_N}}{A^{(N+1)(\frac{d}{2}-1)}} \right). \quad (6.19)$$

(Note that this equivalence depends on  $\eta > 0$ ). We are now able to apply Lemma 3 in (6.19) since  $hL^2 = L^{3/4} \gg (thL^2)^{1/4} = O(L^{1/2})$  for any  $t \in [(\eta/h), (R^2/h)]$ . We thus write,

$$I_L^2(\phi) \underset{L \rightarrow \infty}{\sim} h \sum_{t=(\eta/h)}^{(R^2/h)-1} (th)^{(N+1)(\frac{d}{2}-1)} (\gamma_{N+1,d} d\sigma(\Omega_0) \dots d\sigma(\Omega_N)) .$$

Treating the sum in  $t$  as a Riemann sum now gives,

$$\begin{aligned} I_L^2(\phi) &\underset{L \rightarrow \infty}{\sim} \left( \int_{\theta=\eta}^{R^2} \theta^{(N+1)(\frac{d}{2}-1)} d\theta \right) (\gamma_{N+1,d} d\sigma(\Omega_0) \dots d\sigma(\Omega_N)) \\ &= 2 \left( \int_{\theta=\sqrt{\eta}}^R \theta^{(N+1)(d-2)+1} d\theta \right) (\gamma_{N+1,d} d\sigma(\Omega_0) \dots d\sigma(\Omega_N)) , \quad (6.20) \end{aligned}$$

where again the equivalence depends on  $\eta > 0$ .

*Last step: conclusion*

The estimate (6.18) together with the equivalence (6.20) are now enough to conclude that for a general smooth and decaying  $\phi$ , the ‘‘Riemann sum’’  $I_L(\phi)$  goes to,

$$2\gamma_{N+1,d} \int_{\theta=0}^{\infty} \theta^{(N+1)(d-2)+1} \int_{\mathbb{S}^{(d-1)(N+1)}} \phi(\theta \mathbf{k}_0, \dots, \theta \mathbf{k}_N) d\sigma(\mathbf{k}_0) \dots d\sigma(\mathbf{k}_N) d\theta ,$$

as  $L \rightarrow \infty$ . Theorem 2 is now proved.  $\square$

## 7 Proof of the assumption **(A)** in dimensions 4, 5, and more

### 7.1 The case $d \geq 5$

In this section we prove the following,

**Lemma 4** *Let  $d \geq 5$ . Then, for any  $l \geq 0$ , and for any  $0 < \delta < 1$ , the limit  $\gamma_{l,d}$  in **(A)** exists. Besides, we have the explicit value,*

$$\begin{aligned} \gamma_{l,d} &= \left( \frac{\Gamma(d/2)}{\Gamma(3/2)^d} \right)^l \sum_{\substack{q_1, \dots, q_l \\ q_i \in \mathbb{N}^*, \forall i}} \sum_{\substack{a_1, \dots, a_l \\ a_i \in [1, q_i], \forall i \\ \gcd(a_i, q_i) = 1, \forall i}} \mathbf{1} \left[ \frac{a_1}{q_1} + \dots + \frac{a_l}{q_l} \in \mathbb{Z} \right] \\ &\quad \times \left( \frac{S(q_1, a_1)}{q_1} \dots \frac{S(q_l, a_l)}{q_l} \right)^d , \quad (7.21) \end{aligned}$$

where the notation (2.26) is used. Finally, we have the bound,

$$\gamma_{l,d} \leq C(d)^l. \quad (7.22)$$

**Remark 13** As already mentioned in the introduction, a standard estimate on Gauss' sums (see [Gr]) gives that  $|S(q, a)| \leq Cq^{1/2}$ . Hence we have the obvious bound,

$$\left| \sum_{\substack{a_1, \dots, a_l \\ a_i \in [1, q_i], \forall i \\ \gcd(a_i, q_i) = 1, \forall i}} \mathbf{1} \left[ \frac{a_1}{q_1} + \dots + \frac{a_l}{q_l} \in \mathbb{Z} \right] \left( \frac{S(q_1, a_1)}{q_1} \dots \frac{S(q_l, a_l)}{q_l} \right)^d \right| \\ \leq C^l (q_1 \dots q_l)^{-\frac{d}{2}+1},$$

implying both the convergence of the series in  $q_1, \dots, q_l$  in (7.21) when  $d \geq 5$  and the bound (7.22).  $\square$

#### Proof of Lemma 4

We already noticed (see (6.5)) the relation,

$$\gamma_{l,d} = \left( \frac{\Gamma(3/2)^d}{\Gamma(d/2)} \right)^l \lim_{A \rightarrow \infty} \frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^l, \quad (7.23)$$

so that the mere limit on the right-hand-side of (7.23) has to be computed.

Now, we recall the value of the singular series (see (2.25)),

$$\mathfrak{S}(A) = \sum_{q \in \mathbb{N}^*} \sum_{\substack{a=1 \\ \gcd(a, q) = 1}}^q \left( \frac{S(q, a)}{q} \right)^d \exp \left( -2i\pi \frac{aA}{q} \right).$$

We are thus in position to compute,

$$\frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(A)^l \\ = \sum_{\substack{q_1, \dots, q_l \\ q_i \in \mathbb{N}^*, \forall i}} \sum_{\substack{a_1, \dots, a_l \\ a_i \in [1, q_i], \forall i \\ \gcd(a_i, q_i) = 1, \forall i}} \left( \frac{S(q_1, a_1)}{q_1} \dots \frac{S(q_l, a_l)}{q_l} \right)^d \\ \times \frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \exp \left( -2i\pi \left[ \frac{a_1}{q_1} + \dots + \frac{a_l}{q_l} \right] B \right) \\ \xrightarrow{A \rightarrow \infty} \sum_{\substack{q_1, \dots, q_l \\ q_i \in \mathbb{N}^*, \forall i}} \sum_{\substack{a_1, \dots, a_l \\ a_i \in [1, q_i], \forall i \\ \gcd(a_i, q_i) = 1, \forall i}} \left( \frac{S(q_1, a_1)}{q_1} \dots \frac{S(q_l, a_l)}{q_l} \right)^d \\ \times \mathbf{1} \left[ \frac{a_1}{q_1} + \dots + \frac{a_l}{q_l} \in \mathbb{Z} \right],$$

and the Lemma is proved.  $\square$



## 7.2 The case $d = 4$

In this section we prove the following,

**Lemma 5** *Let  $d = 4$ . Then, for any  $l \geq 0$ , and any  $0 < \delta < 1$ , there exists a constant  $C(\delta)$  such that,*

$$\frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \mathfrak{S}(B)^l \leq (C(\delta)l)^l. \quad (7.24)$$

*In particular, for any given  $0 < \delta < 1$ , there exists a subsequence in  $A$  such that the right-hand-side of (7.24) converges as  $A \rightarrow \infty$ , for any  $l \geq 0$ , so assumption **(A)** is satisfied with  $\delta_0(4) = 1$  up to subsequences in  $A$ .*

### Proof of Lemma 5

The proof is given in several steps.

At first, let us adopt the following notations for convenience: for any function  $f(B)$  depending on the integer parameter  $B$ , we define the following average,

$$\langle f(B) \rangle_{A,\delta} := \frac{1}{1 + A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} f(B). \quad (7.25)$$

Also, we define the function,

$$e(\mathbf{x}) := \exp(2i\pi\mathbf{x}). \quad (7.26)$$

We thus have from its definition (see (2.25)),

$$\mathfrak{S}(B) = \sum_{q \geq 1} \sum_{\substack{a \in [1, q] \\ \gcd(a, q) = 1}} \left( \frac{S(q, a)}{q} \right)^d e\left(-\frac{aB}{q}\right), \quad (7.27)$$

and  $S(q, a)$  is defined in (2.26).

*First step: decomposing  $\mathfrak{S}$  into a partial sum and a remainder term*

Let  $Q \in \mathbb{N}^*$  be a given truncation parameter. We decompose the series defining  $\mathfrak{S}$  into the contribution of  $q$ 's satisfying  $q \leq Q$  and a remainder term, as follows,

$$\begin{aligned} \mathfrak{S}(B) &= \sum_{1 \leq q \leq Q} \sum_{\substack{a \in [1, q] \\ \gcd(a, q) = 1}} \left( \frac{S(q, a)}{q} \right)^d e\left(-\frac{aB}{q}\right) \\ &\quad + \sum_{q \geq Q} \sum_{\substack{a \in [1, q] \\ \gcd(a, q) = 1}} \left( \frac{S(q, a)}{q} \right)^d e\left(-\frac{aB}{q}\right) \\ &=: \mathfrak{S}_Q(B) + R_Q(B). \end{aligned} \quad (7.28)$$

This serves as a definition for the terms  $\mathfrak{S}_Q(B)$  and  $R_Q(B)$ .

We wish to bound uniformly in  $A$  the average  $\langle \mathfrak{S}(B)^l \rangle_{A,\delta}$  for any integer  $l$ . According to the above decomposition, the proof is obtained below by proving on the one hand that,

$$\langle \mathfrak{S}_A(B)^l \rangle_{A,\delta} \leq (C(\delta)l)^l, \quad (7.29)$$

for any  $l$ , and that,

$$\langle R_A(B)^l \rangle_{A,\delta} \leq C(\varepsilon)^l (\log A)^l A^{-1+\varepsilon} \xrightarrow{A \rightarrow \infty} 0, \quad (7.30)$$

for any  $l$ , where the truncation level  $Q$  is chosen equal to  $A$  in (7.29) and (7.30). Lemma 5 is obviously proved once (7.29) and (7.30) are established.

*Second step: estimating  $R_A$*

Following [CP], we first claim that the following bound holds,

$$R_A(B) \leq C(\varepsilon)\tau(B) A^{-1+\varepsilon}, \quad (7.31)$$

where as usual  $\tau(B)$  denotes the number of divisors of  $B$ .

Assuming (7.31) for the moment, we first prove that this estimate implies (7.30). Indeed, it is well-known (see [Te]) that  $\tau(B)$  satisfies,

$$\tau(B) \leq C \log B.$$

This together with (7.31) gives,

$$\langle R_A^l(B) \rangle_{A,\delta} \leq C^l (\log A)^l A^{-1+\varepsilon} \xrightarrow{A \rightarrow \infty} 0. \quad (7.32)$$

We now turn to the proof of (7.31). It relies on the simple observation (See [Ay], or also [CP]),

$$S(q, a) = \left( \frac{a}{q} \right) \sqrt{q} \lambda_q, \quad (7.33)$$

where  $\left( \frac{a}{q} \right)$  is the so-called Jacobi-Legendre symbol of  $a$  and  $q$ , and  $\lambda_q$  is a sequence in  $q$ , whose explicit value can be obtained (see [CP]). The important point to notice is,

$$\left( \frac{a}{q} \right) := \pm 1, \quad \text{and } |\lambda_q| \leq C. \quad (7.34)$$

Therefore, when  $d = 4$ , we obtain the following simplified value of the singular series  $\mathfrak{S}$ ,

$$\mathfrak{S}(B) = \sum_{q \geq 1} \frac{\lambda_q^4}{q^2} c_q(B), \quad (7.35)$$

where  $c_q(B)$  is the so-called Ramanujan sum, defined as,

$$c_q(B) := \sum_{\substack{a=1 \\ \gcd(a, q)=1}}^q e\left(-\frac{aB}{q}\right). \quad (7.36)$$

We turn to estimating  $\mathfrak{S}$  or more precisely the associated remainder term  $R_A$  under the form (7.35). This relies on estimating  $c_q$ . It is well-known (see [Te]) that  $c_q(B)$  actually admits the following value,

$$c_q(B) = \frac{\varphi(q)\mu\left(\frac{q}{\gcd(q, B)}\right)}{\varphi\left(\frac{q}{\gcd(q, B)}\right)}, \quad (7.37)$$

where  $\varphi(q)$  is the so-called Euler totient function, and  $\mu$  is the Möbius function. We do not recall the definitions of these functions but rather recall some basic bounds on them. Indeed we have (see [Te]),

$$C(\varepsilon)q^{1-\varepsilon} \leq \varphi(q) \leq q, \quad (7.38)$$

and,

$$|\mu(q)| \leq C. \quad (7.39)$$

Hence, putting (7.39), (7.38), and (7.37) together gives,

$$\begin{aligned} |c_q(B)| &\leq C \frac{\varphi(q)}{\varphi\left(\frac{q}{\gcd(q, B)}\right)} \\ &\leq C(\varepsilon) \frac{q}{q^{1-\varepsilon}} (\gcd(q, B))^{1-\varepsilon} = C(\varepsilon)q^\varepsilon (\gcd(q, B))^{1-\varepsilon}, \end{aligned}$$

so that we obtain in (7.35),

$$\begin{aligned} |R_A(B)| &\leq \sum_{q \geq A} C(\varepsilon)q^{-2+\varepsilon} (\gcd(q, B))^{1-\varepsilon} = C(\varepsilon) \sum_{\substack{t|B, t|q \\ q \geq A}} q^{-2+\varepsilon} t^{1-\varepsilon} \\ &\leq C(\varepsilon) \sum_{\substack{t|B, t|q \\ q \geq A}} q^{-2+\varepsilon} t = C(\varepsilon) \sum_{t|B} t \left( \sum_{\substack{q=0 \pmod t \\ q \geq A}} q^{-2+\varepsilon} \right) \\ &= C(\varepsilon) \sum_{t|B} t \left( \sum_{q \geq A/t} t^{-2+\varepsilon} q^{-2+\varepsilon} \right) \\ &\leq C(\varepsilon) \left( \sum_{t|B} 1 \right) A^{\varepsilon-1}, \end{aligned}$$

and (7.31) is proved.

*Fourth step: estimating the partial sum  $\mathfrak{S}_A$*

For a given integer  $l$ , we first write,

$$\begin{aligned} \langle \mathfrak{S}_A^l(B) \rangle_{A,\delta} &= \frac{1}{1+A^{1-\delta}} \sum_{B=A}^{A+A^{1-\delta}} \sum_{1 \leq q_1, \dots, q_l \leq A} \sum_{\substack{a_1, \dots, a_l \\ a_i \in \llbracket 1, q_i \rrbracket, \forall i \\ \gcd(a_i, q_i) = 1}} \left( \prod_{i=1}^l \frac{S(a_i, q_i)}{q_i} \right)^4 \\ &\quad \times e \left( - \left[ \sum_{i=1}^l \frac{a_i}{q_i} \right] B \right). \end{aligned}$$

Taking (7.33) into account, we can upper-bound,

$$\begin{aligned} & \left| \langle \mathfrak{S}_A^l(B) \rangle_{A,\delta} \right| \\ &= \frac{1}{1+A^{1-\delta}} \left| \sum_{B=A}^{A+A^{1-\delta}} \sum_{1 \leq q_1, \dots, q_l \leq A} \sum_{\substack{a_1, \dots, a_l \\ a_i \in \llbracket 1, q_i \rrbracket, \forall i \\ \gcd(a_i, q_i) = 1}} \left( \prod_{i=1}^l \frac{\lambda_{q_i}^4}{q_i^2} \right) e \left( - \left[ \sum_{i=1}^l \frac{a_i}{q_i} \right] B \right) \right| \\ &\leq C^l \sum_{1 \leq q_1, \dots, q_l \leq A} \frac{1}{q_1^2 \cdots q_l^2} \times g_{q_1, \dots, q_l}(A, \delta), \end{aligned} \quad (7.40)$$

up to introducing the quantity,

$$g_{q_1, \dots, q_l}(A, \delta) := \sum_{\substack{a_1, \dots, a_l \\ a_i \in \llbracket 1, q_i \rrbracket, \forall i \\ \gcd(a_i, q_i) = 1}} \frac{1}{1+A^{1-\delta}} \left| \sum_{B=A}^{A+A^{1-\delta}} e \left( - \left[ \sum_{i=1}^l \frac{a_i}{q_i} \right] B \right) \right|. \quad (7.41)$$

Now, using that  $g$  is symmetric in  $(q_1, \dots, q_l)$ , we may readily upper bound in (7.40),

$$\left| \langle \mathfrak{S}_A^l(B) \rangle_{A,\delta} \right| \leq C^l \sum_{1 \leq q_1 \leq \dots \leq q_l \leq A} \frac{g_{q_1, \dots, q_l}(A, \delta)}{q_1^2 \cdots q_l^2}. \quad (7.42)$$

There remains therefore to estimate  $g$  as it is defined in (7.41).

*Fifth step: estimating  $g_{q_1, \dots, q_l}(A, \delta)$*

For any given values of the  $q_i$ 's, the function  $g$  is defined as a sum over all integers  $a_i \in \llbracket 1, q_i \rrbracket$  such that  $\gcd(a_i, q_i) = 1$  ( $i = 1, \dots, l$ ). Let  $G_{q_1, \dots, q_l}$  denote the set of all such  $a_i$ 's. We are now naturally led to estimate differently several contributions arising from the following subsets  $G_{q_1, \dots, q_l}$ .

*a- First case: contribution of the subset  $\frac{a_1}{q_1} + \dots + \frac{a_l}{q_l} \in \mathbb{Z}$*

First of all, we easily estimate the cardinality of such  $a_i$ 's,

$$\# \left\{ (a_1, \dots, a_l) \in G_{q_1, \dots, q_l} \text{ s.t. } \frac{a_1}{q_1} + \dots + \frac{a_l}{q_l} \in \mathbb{Z} \right\} \leq q_2 \cdots q_l.$$

(this is true at least if  $A \geq 2$ , which is the case here). For this reason, the corresponding contribution to  $g_{q_1, \dots, q_l}(A, \delta)$  is bounded by,

$$\leq \frac{q_2 \cdots q_l}{1 + A^{1-\delta}} (1 + A^{1-\delta}) = q_2 \cdots q_l. \quad (7.43)$$

*b- Second case: contribution of the set  $\frac{a_1}{q_1} + \cdots + \frac{a_l}{q_l} \notin \mathbb{Z}$*

In this case we wish to use the easy estimate,

$$\frac{1}{1 + A^{1-\delta}} \left| \sum_{B=A}^{A+A^{1-\delta}} e \left( - \left[ \sum_{i=1}^l \frac{a_i}{q_i} \right] B \right) \right| \leq \inf \left( 1, \frac{2}{(1 + A^{1-\delta}) \left\| \sum_{i=1}^l \frac{a_i}{q_i} \right\|} \right), \quad (7.44)$$

where  $\|z\| := \min_{n \in \mathbb{Z}} |z - n|$ . For this reason we need to further subdivide the present case according to whether the quantity

$$\left\| \sum_{i=1}^l (a_i/q_i) \right\|$$

is “large” or “small”, as follows.

*b-1- First sub-case: contribution of the set  $\left\| \sum_{i=1}^l \frac{a_i}{q_i} \right\| \geq \frac{1}{q_1^{1-(\delta/2)}}$*

The cardinality of  $l$ -tuples  $(a_1, \dots, a_l) \in G_{q_1, \dots, q_l}$  satisfying  $\left\| \sum_{i=1}^l \frac{a_i}{q_i} \right\| \geq \frac{1}{q_1^{1-(\delta/2)}}$  is trivially bounded by  $q_1 \cdots q_l$ . For this reason, the corresponding contribution to  $g_{q_1, \dots, q_l}(A, \delta)$  is bounded by,

$$\leq q_1 \cdots q_l \times \frac{q_1^{1-(\delta/2)}}{1 + A^{1-\delta}} = \frac{q_1^{2-(\delta/2)} q_2 \cdots q_l}{1 + A^{1-\delta}}. \quad (7.45)$$

*b-2- Second sub-case: contribution of the set  $\left\| \sum_{i=1}^l \frac{a_i}{q_i} \right\| \leq \frac{1}{q_1^{1-(\delta/2)}}$*

It is known (see [Nie], [Gre], or also [Pl], and [Te]) that the quantity  $a_1/q_1$  is “uniformly distributed” in the interval  $[0, 1]$  as  $a_1$  varies with the constraints  $1 \leq a_1 \leq q_1$  and  $\gcd(a_1, q_1) = 1$ . As a consequence, it is readily seen that there exists a constant  $C(\delta)$  such that for any  $z \in \mathbb{R}$ , we have,

$$\frac{\#\left\{ a_1 \in \llbracket 1, q_1 \rrbracket \text{ s.t. } \gcd(a_1, q_1) = 1 \text{ and } \left\| \frac{a_1}{q_1} - z \right\| \leq \frac{1}{q_1^{1-(\delta/2)}} \right\}}{\#\{a_1 \in \llbracket 1, q_1 \rrbracket \text{ s.t. } \gcd(a_1, q_1) = 1\}} \leq C(\delta) \frac{1}{q_1^{1-(\delta/2)}}. \quad (7.46)$$

(Indeed, the left-hand-side of (7.46) behaves like  $2/q_1^{1-\delta/2}$  as  $q_1 \rightarrow \infty$ ). In other words, the proportion of  $a_1$ 's satisfying the additional constraint  $\|a_1/q_1 - z\| \leq 1/q_1^{1-(\delta/2)}$  has the same size as the interval  $[z - q_1^{(\delta/2)-1}, z + q_1^{(\delta/2)-1}]$ . Now, (7.46) implies that, for any  $z \in \mathbb{R}$ ,

$$\begin{aligned} & \# \left\{ a_1 \in \llbracket 1, q_1 \rrbracket \text{ s.t. } \gcd(a_1, q_1) = 1 \text{ and } \left\| \frac{a_1}{q_1} - z \right\| \leq \frac{1}{q_1^{1-(\delta/2)}} \right\} \\ & \leq C(\delta) \frac{1}{q_1^{1-(\delta/2)}} \times q_1 = C(\delta) q_1^{\delta/2}, \end{aligned}$$

and we readily deduce that,

$$\# \left\{ (a_1, \dots, a_l) \in G_{q_1, \dots, q_l} \text{ s.t. } \left\| \sum_{i=1}^l \frac{a_i}{q_i} \right\| \leq \frac{1}{q_1^{1-(\delta/2)}} \right\} \leq C(\delta) q_1^{\delta/2} q_2 \dots q_l. \quad (7.47)$$

From (7.47) and (7.44), it is easily deduced that the contribution of the  $a_i$ 's such that  $\|\sum_{i=1}^l a_i/q_i\| \leq 1/q_1^{1-(\delta/2)}$  to the sum defining  $g_{q_1, \dots, q_l}(A, \delta)$  is bounded by,

$$\leq C(\delta) q_1^{\delta/2} q_2 \dots q_l. \quad (7.48)$$

*Sixth step: the final upper bound on  $\mathfrak{S}_A$*

Now, putting (7.42), (7.43), (7.45), and (7.48) together gives,

$$\begin{aligned} & \left| \langle \mathfrak{S}_A^l(B) \rangle_{A, \delta} \right| \\ & \leq C^l \sum_{1 \leq q_1 \leq \dots \leq q_l \leq A} \frac{q_1^{2-(\delta/2)} q_2 \dots q_l}{A^{1-\delta} q_1^2 \dots q_l^2} + C(\delta)^l \sum_{1 \leq q_1 \leq \dots \leq q_l \leq A} \frac{q_1^{\delta/2} q_2 \dots q_l}{q_1^2 \dots q_l^2} \\ & \leq C(\delta)^l \sum_{q_1=1}^A \left( \frac{q_1^{-(\delta/2)} (\log q_1)^l}{A^{1-\delta}} + q_1^{-2+(\delta/2)} (\log q_1)^l \right) \\ & \leq (C(\delta)l)^l \left( \frac{A^{1-(\delta/2)} (\log A)^l}{A^{1-\delta}} + 1 \right) \\ & \leq (C(\delta)l)^l. \end{aligned} \quad (7.49)$$

*Last step: conclusion*

Putting estimates (7.32) and (7.49) together gives,

$$\langle \mathfrak{S}^l(B) \rangle_{A, \delta} \sim_{A \rightarrow \infty} \langle \mathfrak{S}_A^l(B) \rangle_{A, \delta} \leq (C(\delta)l)^l.$$

This proves Lemma 5. □

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