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A Rigorous Model Sustaining van Hove's Phenomenon

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Abstract. An exactly solvable model is considered for which we prove the validity of van Hove's perturbative scheme for computing the rate of approach to equilibrium.

Introduction

Some twenty years ago van Hove [1] noticed that for a large class of quantum mechanical, many-body systems showing a dissipative behaviour, the macroscopic size N manifests itself through a characteristic property of the Hamiltonian H , namely: H can be written as $H_0 + \lambda V$ in such a manner that, when computed in a basis for which H_0 is diagonal, the matrix elements $\langle \theta | V^2 | \theta' \rangle$ show a 'diagonal singularity' of order N not present in the matrix elements of V .

To show how this property could plausibly be held responsible for the approach to equilibrium, he used it to support his proposal of a perturbative scheme leading to a Pauli-type master equation which avoided invoking any *ad hoc* repeated random phase ansatz.

Instead of this ansatz van Hove called upon two limiting procedures: i) the infinite-volume limit, in which the spectrum of the unperturbed Hamiltonian H_0 becomes continuous; and ii) the weak coupling limit $\lambda \rightarrow 0$, in which the time t is rescaled in such a manner that $\tau = \lambda^2 t$ remains finite.

The purpose of our paper is to present a simple exactly solvable model, which is yet realistic enough to exhibit precisely the various phenomena anticipated by van Hove. For this model van Hove's prescriptions will, in each step, be actually given a precise mathematical meaning; in particular the above two limiting procedures will be completely brought under control, and van Hove's perturbative scheme will be shown to converge; this dissipative behaviour predicted by van Hove will thus be proven to be a strict consequence of the microscopic dynamics in the limits considered.

The model which we consider is precisely described in Section 1. It consists of quantum particles moving, according to the laws of Hamiltonian mechanics, in a three-dimensional lattice \mathbb{Z}^3 on which scattering impurities are distributed in such a manner that their effect is that of a static stochastic field on \mathbb{Z}^3 . The existence and lattice-translation invariance of the resulting time-evolution for this infinitely extended system are proven in that section, thus giving us control over the first of the two limiting procedures called forth in van Hove's scheme.

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In Section 2 we bring under control the perturbative scheme proposed by van Hove to take into account the long-time cumulative effect of a weak perturbation. The resulting dynamics, expressed in the appropriate time-scale, is shown to be then given by a dissipative semi-group, the generator of which is computed explicitly.

The extension of the results of Section 2 to the time evolution of the extensive observables is described in Section 3, resulting in a Pauli-type master equation of the form predicted by van Hove.

In Section 4 we briefly discuss some physical implications and generalizations of our results.

1. Definition of the Model

Let \mathbb{Z}^3 denote the three-dimensional lattice $\{n = (n^x, n^y, n^z) | n^i \in \mathbb{Z}\}$ and B denote its dual space $\{\theta = (\theta^x, \theta^y, \theta^z) | \theta^i \in [-\pi, \pi]\}$.

The Hilbert space

$$\mathcal{H} = \mathcal{L}^2(\mathbb{Z}^3) = \left\{ f: \mathbb{Z}^3 \rightarrow \mathbb{C} \mid \sum_{n \in \mathbb{Z}^3} |f_n|^2 < \infty \right\}$$

will be the one-particle space of our model. We introduce the momentum representation:

$$f(\theta) = \left(\frac{1}{2\pi} \right)^{3/2} \sum_{n \in \mathbb{Z}^3} e^{i\theta n} f_n$$

with $\theta n = \theta^x n^x + \theta^y n^y + \theta^z n^z$, and the inverse transformation

$$f_n = \left(\frac{1}{2\pi} \right)^{3/2} \int_B d\theta e^{-i\theta n} f(\theta).$$

The model is defined by a ‘random’ Hamiltonian $\tilde{H} = \tilde{H}_0 + \lambda \tilde{V}$ acting on the Fock space $\mathfrak{F}(\mathcal{H})$ (which can be taken to be symmetric or antisymmetric depending on whether the model consists of bosons or of fermions, a choice which we do not need to make here). The free Hamiltonian \tilde{H}_0 is defined in the momentum representation by

$$\tilde{H}_0 = \int_B d\theta \omega(\theta) a^*(\theta) a(\theta)$$

with dispersion law $\omega(\theta) = \theta^2$.

The interaction

$$\tilde{V} = \left(\frac{1}{2\pi} \right)^{3/2} \int_B d\theta \int_B d\theta' v(\theta - \theta') a^*(\theta) a(\theta')$$

is an operator-valued random variable which describes the scattering of the particles by a classical, lattice-translations invariant, Gaussian stochastic field v .

The aim of this section is to give a mathematically meaningful description of the time-evolution for this model.

We first notice that, since \tilde{H} is quadratic in the field operators, the time evolution will be quasi-free and will thus be determined by its restriction to the one-particle space \mathcal{H} .

The (one-particle) free Hamiltonian is then defined by

$$(H_0 f)(\theta) = \omega(\theta) f(\theta)$$

and is bounded, since

$$\|H_0\| = \sup_{\theta \in B} \omega(\theta) = 3\pi^2.$$

In order to be able to define precisely the dynamics of the infinitely extended system, we consider for every finite subset M in \mathbb{Z}^3 the cut-off interaction V^M defined by

$$(V^M f)_n = \chi_n^M v_n f_n$$

where χ_n^M is the characteristic function of M , i.e.

$$\chi_n^M = \begin{cases} 1 & \text{if } n \in M \\ 0 & \text{otherwise;} \end{cases}$$

and $v: \mathbb{Z}^3 \rightarrow \mathbb{R}$ is arbitrary. We notice that this operator is also bounded, since

$$\|V^M\| = \sup_{n \in M} |v_n| < \infty \quad (M \text{ is finite!}).$$

Consequently $H^M = H_0 + \lambda V^M$ is well-defined on $\mathcal{L}^2(\mathbb{Z}^3)$ as a bounded, self-adjoint operator. Let $\{U_t^M | t \in \mathbb{R}\}$ be the continuous, one-parameter unitary group generated by H^M :

$$U_t^M = \exp(-iH^M t).$$

We now give a precise meaning to our assertion that the impurities are randomly distributed on \mathbb{Z}^3 : we consider from now on $\{v_n | n \in \mathbb{Z}^3\}$ as a stochastic field which is assumed to be static, translation-invariant and Gaussian. This field is thus described by the covariance function $\gamma: \mathbb{Z}^3 \times \mathbb{Z}^3 \rightarrow \mathbb{R}$,

$$\langle v_n v_m \rangle = \gamma_{n, m},$$

where we impose on γ to satisfy the following conditions:

- i) $\gamma_{n, m} = g_{|n-m|}$
- ii) $\|g\|_1 = \sum_{n \in \mathbb{Z}^3} |g_n| < \infty$
- iii) $g(\theta) = \left(\frac{1}{2\pi}\right)^{3/2} \sum_{n \in \mathbb{Z}^3} e^{i\theta n} g_n > 0$ for all θ in B .

We then consider $\{v_n | n \in M\}$ as an element of $\mathbb{R}^{|M|}$ (where $|M|$ denotes the number of points in M), and we define on $\mathbb{R}^{|M|}$ the Gaussian measure μ^M by

$$\langle v_n \rangle^M = 0$$

$$\langle v_n v_m \rangle^M = g_{n-m} \quad \text{for all } n, m \text{ in } M.$$

The first of the two limiting procedures considered by van Hove will be controlled, for the model discussed here, by the following proposition, the proof of which will be the aim of this section.

Proposition 1: For every t in \mathbb{R} there exists a function $V_t: B \rightarrow \mathbb{C}$, essentially bounded by 1, such that for every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$:

$$\lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M = \int_B d\theta \varphi^*(\theta) V_t(\theta) \psi(\theta).$$

Before entering into the proof of this proposition, a general methodological remark is in order. The aim of the present paper is to fill the mathematical gaps left in van Hove's proposal and thereby to show that each of its intermediate steps can be given a precise mathematical justification, rather than to give an alternate derivation of his results for the model considered here. We will therefore follow the traditional route of perturbation theory and prove that the convergence of the perturbation expansion can be controlled. This will be achieved by repeated use of the denominated convergence theorem. As far as the above proposition is concerned, the translation invariance of the model will only be used towards the end of the proof, once the existence of the infinite volume limit (with the cut-off removed!) will already have been established. By proceeding in this way we will also prepare naturally the grounds for the material to be presented later in Section 2. In the present paper, we will not touch upon the question of whether the stochastic differential equation aspect of our model could, or could not, be better taken into account by using, in a non-perturbative manner, the methods of functional integration theory.

We first show that the time-evolution, averaged over the Gaussian measure μ^M , exists for each finite cut-off M .

Lemma 1.1: For every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$, every t in \mathbb{R} , and every finite subset M in \mathbb{Z}^3 :

$$\langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M = \sum_{n=0}^{\infty} \langle (\varphi, (U_{\lambda}^M)_t^{(n)} \psi) \rangle^M$$

where

$$(U_{\lambda}^M)_t^{(n)} = (-i\lambda)^n \int_{0 \leq t_1 \leq \dots \leq t_n \leq t} dt_n \dots \int dt_1 V_{t_n}^M \dots V_{t_1}^M$$

and

$$V_{t_i}^M = U_{-t_i}^0 V^M U_{t_i}^0.$$

Proof: By the dominated convergence theorem, the lemma follows from the following premises which are easily established:

i) with $v^M = \sup_{n \in M} |v_n|$

$$\langle \exp(\lambda t v^M) \rangle^M = \int d\mu^M \exp(\lambda t v^M)$$

exists since g is strictly positive;

ii) the Dyson perturbation expansion

$$U_{-t}^0 U_t^M = \sum_{n=0}^{\infty} (U_{\lambda}^M)_t^{(n)}$$

converges in the norm topology; and we actually have

iii) $\|(U_{\lambda}^M)_t^{(n)}\| \leq \frac{1}{n!} (\lambda t v^M)^n, \text{ q.e.d.}$

For the proof of the proposition we will need two technical lemmata which we now establish.

Lemma 1.2: For every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$ with $\|\varphi\| = 1$, every t in \mathbb{R}^+ , every finite sequence $0 \leq t_1 \leq \dots \leq t_n \leq t$, and every finite subset M in $\mathbb{Z}^3: \langle (\varphi, V_{t_n}^M \dots V_{t_1}^M \psi) \rangle^M = 0$ unless n is even, in which case:

$$|\langle (\varphi, V_{t_{2n}}^M \dots V_{t_1}^M \psi) \rangle^M| \leq \frac{(2n)!}{n! 2^n} \|g\|_1^n \sum_{k_{2n} \dots k_0 \in M} \prod_{j=2}^{2n} |u_{t_j - t_{j-1}}(k_j - k_{j-1})| |u_{t_1}(k_1 - k_0)| |\psi_{k_0}|$$

where

$$u_t(k) = \left(\frac{1}{2\pi}\right)^3 \int_B d\theta \exp(-i[\omega(\theta)t + k\theta]).$$

Proof: From the very definition of the operator $V_{t_i}^M$ we have

$$\langle (\varphi, V_{t_n}^M \dots V_{t_1}^M \psi) \rangle^M = \sum_{k_n \dots k_0 \in M} \varphi_{t_n, k_n}^* \langle v_{k_n} \dots v_{k_1} \rangle^M.$$

$$u_{t_n - t_{n-1}}(k_n - k_{n-1}) \dots u_{t_2 - t_1}(k_2 - k_1) u_{t_1}(k_1 - k_0) \psi_{k_0}$$

with

$$\varphi_{t, k} = (U_t^0 \varphi)_k = (\hat{\psi}, \varphi_t) \text{ where } \hat{\psi}(\theta) = \left(\frac{1}{2\pi}\right)^{3/2} e^{-ik\theta};$$

clearly then

$$|\varphi_{t, k}| \leq \|\varphi_t\| \|\hat{\psi}\| = \|\varphi\| \|\hat{\psi}\| = 1.$$

On the other hand, the properties of the Gaussian measure μ^M imply immediately that $\langle v_{k_n} \dots v_{k_1} \rangle^M$ vanishes unless n is even, in which case we have

$$\langle v_{k_{2n}} \dots v_{k_1} \rangle^M = \sum \prod g_{k_i - k_j}$$

where the sum \sum runs over the $(2n - 1)!!$ possible pairings of the $2n$ indices $\{k_{2n} \dots k_1\}$, and where the product \prod runs, for each pairing, over the n pairs of indices occurring in that pairing. We thus get the majorization

$$|\langle v_{k_{2n}} \dots v_{k_1} \rangle^M| \leq \frac{2n!}{n! 2^n} \|g\|_1^n$$

for which the lemma follows immediately. q.e.d.

This lemma will be used in conjunction with the following result:

Lemma 1.3: For every t in \mathbb{R}^+ there exists a finite constant C_t such that for all $\tau_j = t_j - t_{j-1}$, $j = 2, \dots, 2n$, with $0 \leq t_1 \leq \dots \leq t_{2n} \leq t$, one has $\|u_{\tau_j}\|_1 \leq C_t$.

Proof: Upon integrating by part twice, one checks that in one dimension, we have for $k \neq 0$,

$$\begin{aligned} & \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp(-i[\theta^2 \tau + k\theta]) \\ &= \frac{i\tau}{\pi k^2} \left[-2\pi \exp(-i\pi^2 \tau) + \int_{-\pi}^{\pi} d\theta (1 - 2i\theta^2 \tau) \exp(-i[\theta^2 \tau + k\theta]) \right], \end{aligned}$$

so that there exists finite constants $\alpha, \beta \geq 0$, independent of τ , such that

$$\frac{1}{2\pi} \left| \int_{-\pi}^{\pi} d\theta \exp(-i[\theta^2 \tau + k\theta]) \right| \leq \frac{1}{k^2} (\alpha\tau + \beta\tau^2);$$

for $k = 0$ we have

$$\frac{1}{2\pi} \left| \int_{-\pi}^{\pi} d\theta \exp(-i\theta^2 \tau) \right| \leq 1$$

and thus

$$\sum_{k \in \mathbb{Z}} \frac{1}{2\pi} \left| \int_{-\pi}^{\pi} d\theta \exp(-i[\theta^2 \tau + k\theta]) \right| \leq 1 + C(\alpha\tau + \beta\tau^2).$$

The lemma then follows from the fact that the right-hand side of this expression is an increasing function of τ . We have indeed:

$$C_t = [1 + C(\alpha t + \beta t^2)]^3 \quad \text{q.e.d.}$$

Proof of Proposition 1: By Lemma 1.3, all the $u_i(\cdot)$ appearing in Lemma 1.2 are in \mathcal{L}^1 ; hence the convolution product

$$\sum_{k_{2n} \dots k_0 \in M} \prod_{j=2}^{2n} |u_{t_j - t_{j-1}}(k_j - k_{j-1})| |u_{t_1}(k_1 - k_0)| |\psi k_0|$$

is convergent and bounded by $C_t^{2n} \|\psi\|_1$ for $\psi \in \mathcal{L}^1(\mathbb{Z}^3)$ as $M \rightarrow \mathbb{Z}^3$. Upon inserting this into Lemma 1.2, we get

$$|\langle (\varphi, V_{t_{2n}}^M \dots V_{t_1}^M \psi) \rangle^M| \leq \frac{2n!}{n! 2^n} \|g\|_1^n C_t^{2n} \|\psi\|_1$$

which is uniform in M . Consequently the following two limits exist and are equal

$$\lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, (U_\lambda^M)^{(2n)} \psi) \rangle^M = (-i\lambda)^{2n} \int_{0 \leq t_1 \leq \dots \leq t_{2n} \leq t} dt_{2n} \dots \int dt_1 \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, V_{t_{2n}}^M \dots V_{t_1}^M \psi) \rangle^M.$$

Moreover

$$|\langle (\varphi, (U_\lambda^M)^{(2n)} \psi) \rangle^M| \leq \|\varphi\| \|\psi\|_1 \frac{1}{n!} \left(\frac{\lambda^2}{2} \|g\|_1 t^2 C_t^2 \right)^n$$

where the right-hand side is the general term of a series which converges for all t in \mathbb{R} , this majorization being uniform in M . We can therefore use the dominated convergence theorem to conclude the existence of the limit

$$\lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M \equiv B_t(\varphi, \psi), \quad \text{for } \psi \in \mathcal{L}^1(\mathbb{Z}^3);$$

this sesquilinear form in φ, ψ is thus obtained as the limit of the sesquilinear forms:

$$B_t^M(\varphi, \psi) = \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M$$

which are bounded by $\|\varphi\| \|\psi\|$ uniformly in M . Consequently $B_t(\varphi, \psi)$ is also bounded by $\|\varphi\| \|\psi\|$ and there exists an operator V_t on $\mathcal{L}^2(\mathbb{Z}^3)$, bounded by 1, and such that

$$\lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M = (\varphi, V_t \psi).$$

For every translation a in \mathbb{Z}^3 , let U_a be the unitary operator defined by $(U_a f)_n = f_{n+a}$, and write $M + a$ for the set $\{m + a | m \in M\}$. We clearly have, in view of the lattice translation invariance of our measure μ :

$$B_t^{M+a}(\varphi, \psi) = B_t^M(U_a \varphi, U_a \psi)$$

from which follows

$$B_t(\varphi, \psi) = B_t(U_a \varphi, U_a \psi)$$

and thus V_t commutes with U_a for every a in \mathbb{Z}^3 . Consequently $(V_t f)(\theta) = V_t(\theta) f(\theta)$ for every f in $\mathcal{L}^2(\mathbb{Z}^3)$; since

$$\text{ess sup}_{\theta \in B} |V_t(\theta)| = \|V_t\| \leq 1$$

this concludes the proof of Proposition 1. q.e.d.

2. Van Hove's Long-Time, Weak-Coupling Limit

The purpose of this section is to control van Hove's perturbative scheme in the so-called $\lambda^2 t$ limit for the model considered in Section 1. Specifically, we will present now a complete proof of the following result:

Proposition 2: There exists $\tau_0 > 0$ such that for each fixed τ in $[0, \tau_0]$, and every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$:

$$\lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M = \int_B d\theta \varphi^*(\theta) S_t(\theta) \psi(\theta).$$

where

$$S_\tau(\theta) = \exp(-[\Gamma(\theta) + i\Delta(\theta)]\tau)$$

with

$$\Gamma(\theta) = \pi \int d\theta' W(\theta', \theta) \delta(\omega(\theta') - \omega(\theta))$$

$$\Delta(\theta) = \int d\theta' W(\theta', \theta) (\omega(\theta) - \omega(\theta'))^{-1}$$

$$W(\theta', \theta) = \left(\frac{1}{2\pi}\right)^{3/2} g(\theta - \theta').$$

In order to bring the form of the contractive semi-group $\{S_\tau | \tau \in \mathbb{R}^+\}$ into immediate contact with van Hove's notation, we notice the following property of the kernel $W(\theta', \theta)$.

Lemma 2.1: For every operator A on $\mathcal{L}^2(\mathbb{Z}^3)$ such that $(Af)(\theta) = A(\theta)f(\theta)$ for every f in $\mathcal{L}^2(\mathbb{Z}^3)$, the operator VAV , averaged over the Gaussian measure, is given by the kernel:

$$\lim_{M \rightarrow \mathbb{Z}^3} \langle V^M A V^M \rangle^M(\theta, \theta') = \delta(\theta - \theta') \int d\theta'' A(\theta'') W(\theta'', \theta).$$

Proof:

$$\lim_{M \rightarrow \mathbb{Z}^3} \langle V^M A V^M \rangle^M(\theta, \theta') = \int d\theta'' A(\theta'') \langle v(\theta, \theta'') v(\theta'', \theta') \rangle$$

with

$$\begin{aligned} \langle v(\theta, \theta'') v(\theta'', \theta') \rangle &= \left(\frac{1}{2\pi}\right)^6 \sum_{n \in \mathbb{Z}^3} \sum_{m \in \mathbb{Z}^3} \exp(i[(\theta - \theta'')n + (\theta'' - \theta')m]) \langle v_n v_m \rangle \\ &= \left(\frac{1}{2\pi}\right)^{9/2} \sum_{n \in \mathbb{Z}^3} \exp(i(\theta - \theta')n) \sum_{k \in \mathbb{Z}^3} \exp(i(\theta' - \theta'')k) g_k \\ &= \left(\frac{1}{2\pi}\right)^{3/2} \delta(\theta - \theta') g(\theta - \theta''). \quad \text{q.e.d.} \end{aligned}$$

We should remark that, together with the fact that $\langle V \rangle = 0$, this lemma precisely expresses that our model satisfies van Hove's celebrated 'diagonal singularity' condition.

The proof of Proposition 2 will be presented as a consequence of the following two lemmata:

Lemma 2.2: There exists a finite constant $C > 0$ such that for every t and λ in \mathbb{R} , every n in \mathbb{Z}^+ and every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$ with $\|\varphi\| = \|\psi\| = 1$:

$$\lim_{M \rightarrow \mathbb{Z}^3} |\langle \varphi, (U_\lambda^M)^{(2n)} \psi \rangle| \leq \frac{(2n-1)!!}{n!} C^n (\lambda^2 t)^n.$$

Lemma 2.3: For every τ in \mathbb{R}^+ , every n in \mathbb{Z}^+ , every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$:

$$\lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, (U_\lambda^M)^{(2n)} \psi) \rangle^M = \frac{1}{n!} \int d\theta \varphi^*(\theta) (-\tau[\Gamma(\theta) + i\Delta(\theta)])^n \varphi(\theta).$$

To prove Lemma 2.2 we will need three technical sublemmata which, for sake of completeness, we state and establish here separately, although the content of the first two might probably be found elsewhere in the literature.

Sublemma 2.4: For every pair A, B of finite Hermitian matrices satisfying $A \geq B > 0$, we have:

$$\text{Det } A \geq \text{Det } B > 0.$$

Proof: Let A be a positive matrix on \mathbb{R}^n and $\{f_i | i = 1, 2, \dots, n\}$ be an orthonormal basis in \mathbb{R}^n ; further, let C be the Hermitian, positive matrix defined by

$$Cf_i = \lambda_i f_i \quad \text{with} \quad \lambda_i = (f_i, Af_i).$$

Since A and C are Hermitian and $f: x \rightarrow \lg x, x \in (0, \infty)$, is concave, we have [2]

$$\text{Tr} \{f(A) - f(C) - (A - C) f'(C)\} \leq 0$$

and thus

$$\text{Tr} \lg A \leq \sum_{i=1}^n (f_i, \lg Cf_i) - \sum_{i=1}^n (f_i, (A - C) f_i) (f_i, f'(C) f_i).$$

Since C^{-1} exists, $(f_i, (A - C) f_i) = 0$ and $(f_i, \lg Cf_i) = \lg(f_i, Af_i)$, we have:

$$\text{Tr} \lg A \leq \sum_{i=1}^n \lg(f_i, Af_i).$$

Moreover, the equality sign holds if $\{f_i\}$ is the orthonormal basis which diagonalizes A . Consequently,

$$\text{Tr} \lg A = \inf_{\{f_i\}} \sum_{i=1}^n \lg(f_i, Af_i).$$

With A and B satisfying the assumptions of the lemma we thus have:

$$\text{Tr} \lg A = \inf_{\{f_i\}} \sum_{i=1}^n (f_i, Af_i) \geq \inf_{\{f_i\}} \sum_{i=1}^n (f_i, Bf_i) = \text{Tr} \lg B.$$

On the other hand, if $\{f_i\}$ is an orthonormal basis diagonalizing A , i.e. $Af_i = a_i f_i$, we have

$$\text{Det } A = \prod_{i=1}^n a_i = \exp \left(\sum_{i=1}^n \lg a_i \right) = \exp \text{Tr} \lg A$$

and thus, since $\exp(\cdot)$ is a monotonically increasing function,

$$\text{Det } A = \exp \text{Tr} \lg A \geq \exp \text{Tr} \lg B = \text{Det } B \quad \text{q.e.d.}$$

Sublemma 2.5: There exists a finite constant $C_1 > 0$ such that for every pair $\{Q, L\}$ constituted of a positive quadratic form Q on \mathbb{R}^n and a linear form L on \mathbb{R}^n , and for every cube $D = \{x = (x_1, \dots, x_n) | x_i \in [-a, a]\}$ in \mathbb{R}^n .

$$\left| \int \dots \int_D dx_1 \dots dx_n \exp(-i[Q(x) + L(x)]) \right| \leq (\text{Det } Q)^{-1/2} C_1^n.$$

Proof: Let Ω be an orthogonal transformation of \mathbb{R}^n which diagonalizes Q and write $y_k = (\Omega x)_k$. We have then

$$\begin{aligned} & \int \dots \int_D dx_1 \dots dx_n \exp(-i[Q(x) + L(x)]) \\ &= \int \dots \int_{\Omega(D)} dy_1 \dots dy_n \exp\left(-i \sum_{k=1}^n (\lambda_k y_k^2 + a_k y_k)\right) \end{aligned}$$

with $\lambda_k > 0$ for $k = 1, 2, \dots, n$.

Let now A be the linear transformation on \mathbb{R}^n defined by the change of variables $y_k \rightarrow z_k = \lambda_k^{1/2} y_k$. The right-hand side of the above expression becomes then:

$$\begin{aligned} & (\text{Det } A)^{-1} \int \dots \int_{A\Omega(D)} dz_1 \dots dz_n \exp\left(-i \sum_{k=1}^n (z_k^2 + b_k z_k)\right) \\ &= (\text{Det } Q)^{-1/2} \int \dots \int_{\Omega^{-1}A\Omega(D)} du_1 \dots du_n \exp\left(-i \sum_{k=1}^n (u_k^2 + c_k u_k)\right) \\ &= (\text{Det } Q)^{-1/2} \prod_{k=1}^n \left(\int_{\alpha_k}^{\beta_k} du_k \exp(-i[u_k^2 + c_k u_k]) \right). \end{aligned}$$

The lemma then follows immediately from the additional remark that

$$\left| \int_{\alpha}^{\beta} du \exp(-i(u^2 + cu)) \right|$$

depends continuously on α and β and is thus bounded by a finite constant $C_1 > 0$, independent of α , β and c since

$$\lim_{\alpha \rightarrow -\infty} \lim_{\beta \rightarrow \infty} \left| \int_{\alpha}^{\beta} dy \exp(-iy^2) \right|$$

exists, as is easily seen by repeated integration by parts. q.e.d.

Sublemma 2.6: For any permutation $\{\theta'_{2n}, \theta'_{2n-1}, \dots, \theta'_1\}$ of the variables $\{(\theta_{2n+1} - \theta_{2n}), (\theta_{2n} - \theta_{2n-1}), \dots, (\theta_2 - \theta_1)\}$ with $\theta_j \in B = [-\pi, \pi]^3$, and for any sequence $0 \leq t_1 \leq \dots \leq t_{2n} \leq t < \infty$, there exists a choice $\{s_{j_l} | l = 1, 2, \dots, n\}$, with $s_{j_l} = t_{j_l} - t_{j_l-1}$,

such that for all φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$ with $\|\varphi\| = \|\psi\| = 1$:

$$\left| \int_B d\theta_{2n+1} \int_B d\theta_{2n} \dots \int_B d\theta_1 \varphi^*(\theta_{2n+1}) \psi(\theta_1) \cdot \exp \left(i \left[\omega(\theta_{2n+1}) t_{2n} - \sum_{k=2}^{2n} \omega(\theta_k) (t_k - t_{k-1}) - \omega(\theta_1) t_1 \right] \right) \cdot \prod_{l=1}^n \langle v(\theta'_{2l}) v(\theta'_{2l-1}) \rangle \right| \leq \prod_{l=1}^n h(s_{j_l})$$

with $h(s) = C_2(s + 1)^{-3/2}$ and $0 < C_2 < \infty$.

Proof: By an argument similar to that which we used in the proof of Lemma 2.1, we have:

$$\langle v(\theta') v(\theta'') \rangle = \left(\frac{1}{2\pi} \right)^{3/2} \delta(\theta' + \theta'') g(\theta'').$$

Consequently, each one of the n terms occurring in the product $\prod_{l=1}^n \langle v(\theta'_{2l}) v(\theta'_{2l-1}) \rangle$ contributes a δ -function. These δ -functions lead to n independent linear relations between $\theta_1, \theta_2, \dots, \theta_{2n+1}$; $\theta_1 = \theta_{2n+1}$ being always one of these relations, a fact which expresses the lattice translation invariance of the model. We can therefore keep, in addition to θ_1 , n independent integration variables $\{\theta_{j_1}, \dots, \theta_{j_n}\}$ chosen amongst $\{\theta_2, \dots, \theta_{2n}\}$, and perform the integrations over the n remaining variables with the help of the δ -functions. Once this is done, the left-hand side of the expression to be majorized in our lemma takes the form

$$\int d\theta_1 \varphi^*(\theta_1) \psi(\theta_1) \exp(i\omega(\theta_1)(t_{2n} - t_1 + \sigma)) \cdot \int d\theta_{j_1} \dots \int d\theta_{j_n} \exp \left(-i \left(\sum_{k,l=1}^n \theta_{j_k} \theta_{j_l} \sigma_{kl} + \sum_{k=1}^n \theta_1 \theta_{j_k} \sigma_k \right) \right) \cdot f(\theta_1, \theta_{j_1}, \dots, \theta_{j_n})$$

where

- i) $\sigma, \sigma_{kl}, \sigma_k$ are linear combinations of the variables $s_j = t_j - t_{j-1}$;
- ii) the quadratic form $Q = \sum_{k,l=1}^n \theta_{j_k} \theta_{j_l} \sigma_{kl}$ is obtained from $\sum_{k=2}^{2n} \omega(\theta_k) s_k$, where the $n - 1$ dependent variables $\{\theta_{j_l} | l = n + 1, \dots, 2n - 1\}$ are expressed as linear functions of the n integration variables $\{\theta_{j_l} | l = 1, 2, \dots, n\}$ and θ_1 is set equal to 0. Thus Q is positive;
- iii) $f(\theta_1, \theta_{j_1}, \dots, \theta_{j_n})$ is a product of n functions $g(\cdot)$, which we can thus write as:

$$\left(\frac{1}{2\pi} \right)^{3n/2} \sum_{m_1, \dots, m_n} g_{m_1} \dots g_{m_n} \exp \left(i \left[\sum_{l=1}^n \theta_{j_l} \alpha_l + \theta_1 \alpha \right] \right)$$

where the α_l, α are linear combinations of the m_k 's.

We have thus that the expression to be majorized is equal to

$$\left(\frac{1}{2\pi}\right)^{3n/2} \int d\theta_1 \varphi^*(\theta_1) \psi(\theta_1) \exp(i\omega(\theta_1)(t_{2n} - t_1 + \sigma)) \\ \sum_{m_1, \dots, m_n} g_{m_1} \dots g_{m_n} \int_B d\theta_{j_1} \dots \int_B d\theta_{j_n} \exp(-i[Q + L](\theta_{j_1}, \dots, \theta_{j_n})),$$

this expression being, in turn, majorized by (see in particular Sublemma 2.5 above)

$$\left(\frac{1}{2\pi}\right)^{3n/2} \|g\|_1^n C_1^{3n} (\text{Det } Q)^{-3/2}.$$

Since, moreover, $Q \geq T$ with $T = \sum_{l=1}^n \theta_{j_l}^2 s_{j_l}$, we have by Sublemma 2.4 above that our expression is majorized by:

$$\left(\frac{1}{2\pi}\right)^{3n/2} \|g\|_1^n C_1^{3n} \prod_{l=1}^n s_{j_l}^{-3/2}.$$

On the other hand, our expression is trivially majorized by:

$$\|g\|_1^n (2\pi)^{3n/2}.$$

The conjunction of these two majorizations produces the desired result. Clearly C_2 is independent of

$$\{\theta'_{2n}, \dots, \theta'_1\} \text{ and } \{t_1, \dots, t_{2n}\}. \text{ q.e.d.}$$

Proof of Lemma 2.2:

$$\lim_{M \rightarrow \mathbb{Z}^3} |\langle (\varphi, (U_\lambda^M)_t^{(2n)} \psi) \rangle^M| = \lambda^{2n} \left| \int_{0 \leq t_1 \leq \dots \leq t_{2n} \leq t} dt_{2n} \dots \int dt_1 \int_B d\theta_{2n+1} \dots \int_B d\theta_1 \varphi^*(\theta_{2n+1}) \psi(\theta_1) \right. \\ \cdot \exp \left(i \left[\omega(\theta_{2n+1}) t_{2n} - \sum_{k=2}^{2n} \omega(\theta_k) (t_k - t_{k-1}) - \omega(\theta_1) t_1 \right] \right) \\ \left. \cdot \langle v(\theta_{2n+1} - \theta_{2n}) v(\theta_{2n} - \theta_{2n-1}) \dots v(\theta_2 - \theta_1) \rangle \right|.$$

Since the measure μ is Gaussian, $\langle v(\cdot) \dots v(\cdot) \rangle$ is the sum of $(2n - 1)!!$ terms of the form

$$\prod_{l=1}^n \langle v(\theta'_{2l}) v(\theta'_{2l-1}) \rangle$$

where $\{\theta'_{2n}, \dots, \theta'_1\}$ is a permutation of the variables $\{(\theta_{2n+1} - \theta_{2n}), (\theta_{2n} - \theta_{2n-1}), \dots, (\theta_2 - \theta_1)\}$. We can therefore use our Sublemma 2.6 to majorize the above expression by:

$$(2n - 1)!! \lambda^{2n} \int_{0 \leq t_1 \leq \dots \leq t_{2n} \leq t} dt_{2n} \dots \int dt_1 \prod_{l=1}^n h(s_{j_l}).$$

The lemma then follows immediately from the fact that there exists a finite constant $C > 0$ such that:

$$\int_0^t ds s^m h(s) \leq t^m \int_0^t ds h(s) \leq t^m \int_0^\infty ds h(s) = Ct^m \quad \text{q.e.d.}$$

We now prove Lemma 2.3 in two steps. We first show that for n fixed the desired result is already obtained from one amongst the $(2n - 1)!!$ permutations which enter in the computation of $\langle v(\theta_{2n+1} - \theta_{2n}) \dots v(\theta_2 - \theta_1) \rangle$. The second step will then consist of proving that the other permutations actually do not contribute in the limit considered.

Sublemma 2.7:

$$\begin{aligned} & \lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} (-i\lambda)^{2n} \int_{0 \leq t_1 \leq \dots \leq t_{2n} \leq t} dt_{2n} \dots \int dt_1 \int_B d\theta_{2n+1} \dots \int_B d\theta_1 \varphi^*(\theta_{2n+1}) \psi(\theta_1) \\ & \cdot \exp \left(i \left[\omega(\theta_{2n+1}) t_{2n} - \sum_{k=2}^{2n} \omega(\theta_k) (t_k - t_{k-1}) - \omega(\theta_1) t_1 \right] \right) \\ & \cdot \prod_{l=1}^n \langle v(\theta_{2l+1} - \theta_{2l}) v(\theta_{2l} - \theta_{2l-1}) \rangle = \frac{(-\tau)^n}{n!} \int_B d\theta \varphi^*(\theta) (\Gamma(\theta) + i\Delta(\theta))^n \psi(\theta). \end{aligned}$$

Proof: From the by now well-known identity

$$\langle v(\theta_{2l+1} - \theta_{2l}) v(\theta_{2l} - \theta_{2l-1}) \rangle = \delta(\theta_{2l+1} - \theta_{2l-1}) W(\theta_{2l}, \theta_{2l+1})$$

we conclude that the expression to be computed is equal to

$$\begin{aligned} & \int_B d\theta \varphi^*(\theta) \psi(\theta) \int_0^t dt_{2n} \int_0^{t_{2n}} dt_{2n-1} f_\theta(t_{2n} - t_{2n-1}) \\ & \cdot \int_0^{t_{2n-1}} dt_{2n-2} \int_0^{t_{2n-2}} dt_{2n-3} f_\theta(t_{2n-2} - t_{2n-3}) \cdot \dots \\ & \cdot \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 f_\theta(t_2 - t_1) \equiv (\varphi, F^{(n)}(t) \psi) \end{aligned}$$

with

$$f_\theta(s) = -\lambda^2 \int_B d\theta' \exp(-i[\omega(\theta') - \omega(\theta)]s) W(\theta', \theta).$$

Since $F^{(n)}(t)$ verifies

$$F_\theta^{(n)}(t) = \int_0^t du \int_0^u dv f_\theta(u - v) F_\theta^{(n-1)}(v)$$

the sublemma is proved by recursion, starting with

$$\lim_{t \rightarrow \infty} \frac{1}{t} F_{\theta}^{(1)}(t) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t du \int_0^u dv f_{\theta}(u-v) = \int_0^{\infty} f_{\theta}(s) ds = -\lambda^2(\Gamma(\theta) + i\Delta(\theta)).$$

We should remark that the permutation considered in this sublemma corresponds exactly to the transition scheme which van Hove, on the basis of his diagonal singularity condition (see our Lemma 2.1), singled out as giving the n th order contribution of his perturbation expansion. This permutation is that for which the integrand of the multiple time-integral is a function only of the successive time differences $\{(t_{2n} - t_{2n-1}), (t_{2n-2} - t_{2n-3}), \dots, (t_2 - t_1)\}$.

For the sake of brevity, we say that $\{(\theta_{2n+1} - \theta_{2n}), (\theta_{2n} - \theta_{2n-1}), \dots, (\theta_2 - \theta_1)\}$, taken in that order, is the 'trivial' permutation of these $2n$ variables; any other permutation will be said to be 'non-trivial'. By a slight refinement of the majorization worked out for Lemma 2.2, we shall now prove that the contribution of every non-trivial permutation vanishes in the limit $t \rightarrow \infty$ with $\lambda^2 t = \tau$ fixed.

Sublemma 2.8: For each n in \mathbb{Z}^+ there exists a finite constant $C_n > 0$ such that for every t and λ in \mathbb{R} , every φ and ψ in $\mathcal{L}^2(\mathbb{Z}^3)$ with $\|\varphi\| = \|\psi\| = 1$, and every non-trivial permutation $\{\theta'_{2n}, \theta'_{2n-1}, \dots, \theta'_1\}$ of the variables $\{(\theta_{2n-1} - \theta_{2n}), \dots, (\theta_2 - \theta_1)\}$ with $\theta_j \in B, j = 1, 2, \dots, 2n+1$:

$$\left| (-i\lambda)^{2n} \int_{0 \leq t_1 \leq \dots \leq t_{2n} \leq t} dt_{2n} \dots \int dt_1 \int_B d\theta_{2n+1} \dots \int_B d\theta_1 \varphi^*(\theta_{2n+1}) \psi(\theta_1) \right. \\ \cdot \exp \left(i \left[\omega(\theta_{2n+1}) t_{2n} - \sum_{k=2}^{2n} \omega(\theta_k) (t_k - t_{k-1}) - \omega(\theta_1) t_1 \right] \right) \\ \left. \cdot \prod_{l=1}^n \langle v(\theta'_{2l}) v(\theta'_{2l-1}) \rangle \right| \leq C_n t^{-1/2} (\lambda^2 t)^n.$$

Proof: The quadratic form Q , which appears in Sublemma 2.6, reduces to $T = \sum_{k=1}^n \theta_{j_k}^2 s_{j_k}$ for the trivial permutation; thus the majorization of Q by T is the best possible if we want to consider simultaneously *all* the permutations $\{\theta'_{2n}, \dots, \theta'_1\}$. We can, nevertheless, improve on this if we exclude from our considerations the trivial permutation, the contribution of which has been evaluated separately in Sublemma 2.7. To this effect, we notice that for every non-trivial permutation $\{\theta'_{2n}, \theta'_{2n-1}, \dots, \theta'_1\}$ it is possible to choose the n variables $\{\theta_{j_l} | l = 1, 2, \dots, n\}$ amongst the $(2n-1)$ variables $\{\theta_k | k = 2, \dots, 2n\}$ in such a manner that, at least, one of the $n-1$ remaining variables, say $\theta_{j_{n+1}}$, is either equal to θ_{j_1} , or is of the form $\theta_{j_{n+1}} = \theta_{j_1} - \theta_{j_2} - \theta_1$. We can thus write

$$Q \geq Q'$$

where Q' is equal to either

$$\theta_{j_1}^2 (s_{j_1} + s_{j_{n+1}}) + \theta_{j_2}^2 s_{j_2} + \dots + \theta_{j_n}^2 s_{j_n}$$

or

$$\theta_{j_1}^2(s_{j_1} + s_{j_{n+1}}) + \theta_{j_2}^2(s_{j_2} + s_{j_{n+1}}) - 2\theta_{j_2}\theta_{j_1}s_{j_{n+1}} + \theta_{j_3}^2s_{j_3} + \dots + \theta_{j_n}s_{j_n}.$$

In both cases

$$\text{Det } Q' \geq (s_{j_1} + s_{j_{n+1}})s_{j_2} \dots s_{j_n}.$$

For the non-trivial permutations we can therefore improve Sublemma 2.6 to

$$\begin{aligned} & \left| \int_B d\theta_{2n+1} \dots \int_B d\theta_1 \varphi^*(\theta_{2n+1}) \psi(\theta_1) \right. \\ & \cdot \exp \left(i \left[\omega(\theta_{2n+1}) t_{2n} - \sum_{k=2}^{2n} \omega(\theta_k)(t_k - t_{k-1}) - \omega(\theta_1) t_1 \right] \right) \\ & \cdot \prod_{l=1}^n \langle v(\theta'_{2l}) v(\theta'_{2l-1}) \rangle \left. \right| \leq h(s_{j_1} + s_{j_{n+1}}) \prod_{l=2}^n h(s_{j_l}). \end{aligned}$$

The sublemma then follows upon noticing that, in the successive time integrations, there will now be one integration of the form

$$\int_0^v duh(u+s) \leq \int_s^\infty duh(u) \leq cs^{-1/2}$$

accounting for the additional $t^{-1/2}$ factor which occurs for every non-trivial permutation.

Proof of Lemma 2.3: We have already seen that

$$\begin{aligned} & \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, (U_\lambda^M)^{(2n)} \psi) \rangle^M \\ & = (-i\lambda)^{2n} \int_{0 \leq t_1 \leq \dots \leq t_{2n} \leq t} dt_{2n} \dots \int dt_1 \int_B d\theta_{2n+1} \dots \int_B d\theta_1 \varphi^*(\theta_{2n+1}) \psi(\theta_1) \\ & \cdot \exp \left(i \left[\omega(\theta_{2n+1}) t_{2n} - \sum_{k=2}^{2n} \omega(\theta_k)(t_k - t_{k-1}) - \omega(\theta_1) t_1 \right] \right) \\ & \cdot \langle v(\theta_{2n+1} - \theta_{2n}) v(\theta_{2n} - \theta_{2n-1}) \dots v(\theta_2 - \theta_1) \rangle. \end{aligned}$$

Since μ is a Gaussian measure, $\langle v(\cdot) \dots v(\cdot) \rangle$ is the sum of $(2n - 1)!!$ terms of the form

$$\prod_{l=1}^n \langle v(\theta'_{2l}) v(\theta'_{2l-1}) \rangle$$

where $\{\theta'_{2n}, \theta'_{2n-1}, \dots, \theta'_1\}$ is a permutation of the $2n$ variables $\{(\theta_{2n+1} - \theta_{2n}), \dots, (\theta_2 - \theta_1)\}$. Sublemma 2.8 shows that, in the limit $t \rightarrow \infty$ with $\lambda^2 t = \tau$ fixed, the contribution of the $(2n - 1)!! - 1$ non-trivial permutations vanishes; hence only the trivial permutation contributes to this limit, a contribution which is computed in Sublemma 2.7. q.e.d.

Proof of Proposition 2: From Lemma 1.1 we know that

$$\lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M = \lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} \lim_{M \rightarrow \mathbb{Z}^3} \sum_{n=0}^{\infty} \langle (\varphi, (U_{\lambda}^M)_t^{(n)} \psi) \rangle^M.$$

We have seen in Lemma 1.2 that $\langle (\varphi, (U_{\lambda}^M)_t^{(n)} \psi) \rangle^M$ vanishes if n is odd, so that the sum carries effectively only over the even n 's. We have further seen in Proposition 1 that the sum and the limit as $M \rightarrow \mathbb{Z}^3$ can be interchanged. Since $(2n-1)!!/n!$ behaves asymptotically for large n as 2^n , Lemma 2.2 shows that the sum and the limit $t \rightarrow \infty$ with $\lambda^2 t = \tau$ fixed can be interchanged; provided that $|\tau| \leq \tau_0 < (2C)^{-1}$. Finally Lemma 2.3 gives the contribution of each summand as the general term of a convergent series summing up to $(\varphi, S_t \psi)$. q.e.d.

Our analysis can actually be used to sharpen the content of Proposition 2 as follows: There exists two constants $\tau_0 > 0$ and $C > 0$ such that for $0 \leq \lambda^2 t \leq \tau_0$

$$\left| \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M - (\varphi, \exp(-[\Gamma + i\Delta] \lambda^2 t) \psi) \right| \leq \lambda C.$$

Indeed: i) we have seen in Sublemma 2.8 that the contribution of the non-trivial permutations is of order $t^{-1/2} \sim \lambda$ for fixed τ ; ii) by slightly refining Sublemma 2.7, it can easily be seen that the rate of convergence of the contribution to the semi-group due to the trivial permutation is also of order $t^{-1/2} \sim \lambda$.

3. Extensive One-Particle Observables

We presented in Section 2 a detailed mathematical study of the matrix elements of the evolution operator in the one-particle space as the simplest illustration of van Hove's phenomenon. One has, of course, to conduct a similar analysis for the time evolution of particle observables. We shall sketch it here for one class of observables of particular physical interest, namely the one-particle observables which are invariant under lattice translations. These observables are of the form:

$$\tilde{A} = \int_B d\theta A(\theta) a^*(\theta) a(\theta).$$

We first define their time evolution, in the interaction picture, for cut-off interactions by

$$\langle A_{\lambda, t}^M \rangle^M = \langle U_t^0 U_{-t}^M A U_t^M U_{-t}^0 \rangle^M$$

with

$$A_{\lambda, t}^M = \sum_{n=0}^{\infty} (A_{\lambda, t}^M)^{(n)}$$

and

$$(A_{\lambda, t}^M)^{(n)} = (-i\lambda)^n \int_{0 \leq t_1 \leq \dots \leq t_n \leq t} dt_n \dots \int dt_1 [V_{t_n}^M, [\dots, [V_{t_1}^M, A]]].$$

We prove along the same lines as those of Section 1 that the infinite-volume limit $M \rightarrow \mathbb{Z}^3$ of $\langle (\varphi, A_{\lambda, t}^M \psi) \rangle^M$ exists for all φ and ψ in \mathcal{H} .

The reader will convince himself that a straightforward extension of the rules established in Section 2 to the commutators expansion of $A_{\lambda, t}^M$, given above leads, term by term, to

$$\lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} \lim_{M \rightarrow \mathbb{Z}^3} \langle (\varphi, A_{\lambda, t}^M \psi) \rangle^M = \int d\theta \varphi^*(\theta) A_\tau(\theta) \psi(\theta)$$

with

$$A_\tau(\theta) = \sum_{n=0}^{\infty} \frac{\tau^n}{n!} (\mathcal{L}^n A)(\theta)$$

where \mathcal{L}^n is the n th iterate of the operator \mathcal{L} defined by

$$(\mathcal{L} A)(\theta) = 2\pi \int d\theta' \delta(\omega(\theta') - \omega(\theta)) W(\theta', \theta) (A(\theta') - A(\theta)).$$

The rules which lead to this result are:

- i) The n th order in the perturbation expansion vanishes for n odd; the multiple-commutator occurring at the $(2n)$ th order is a sum of 2^{2n} terms.
- ii) Each of these 2^{2n} terms is the sum of $(2n - 1)!!$ contributions of the possible pairings. All these contributions, except one, vanish in the $\lambda^2 t$ limit.
- iii) At each even order in the perturbation expansion, all the pairings giving a non-vanishing contribution in the $\lambda^2 t$ limit are identified as those pairings which correspond to the well-ordered sequence of time differences: $\{(t_{2n} - t_{2n-1}), (t_{2n-2} - t_{2n-3}), \dots, (t_2 - t_1)\}$ (see the remark following Sublemma 2.7).
- iv) At order $2n$ in the perturbation expansion, the non-vanishing contributions, in the $\lambda^2 t$ limit, sum up to \mathcal{L}^n .

Therefore the observables which are functions of the momentum operator evolve, in the $\lambda^2 t$ limit, according to a semi-group law whose generator is \mathcal{L} . Equivalently, this is to say that the time evolution, in the $\lambda^2 t$ limit, of the one-particle, lattice-translation invariant observables, is described by the one-particle momentum distribution function $\rho_\tau: B \rightarrow \mathbb{R}^+$, defined by

$$\langle \rho_\tau; A \rangle = \int d\theta \rho_\tau(\theta) A(\theta) = \langle \rho; A_\tau \rangle$$

and satisfying the Pauli-type master equation

$$\frac{d}{d\tau} \rho_\tau = \mathcal{L}^* \rho_\tau$$

where

$$(\mathcal{L}^* \rho)(\theta) = \int_B d\theta' (K(\theta, \theta') \rho(\theta') - K(\theta', \theta) \rho(\theta))$$

with the symmetric kernel

$$K(\theta, \theta') = 2\pi \delta(\omega(\theta') - \omega(\theta)) W(\theta', \theta)$$

in conformity with van Hove's prediction.

4. Discussion of the Results

The main aim of our paper was to show, in detail (see in particular Section 2), how van Hove's perturbation scheme for the computation of the time evolution in the long time, weak coupling limit can be mathematically controlled for a specific model of infinite extension, whose properties mimic those of a generic many-body system. In particular we proved that van Hove's prescription to retain, at each order, only the most divergent diagrams, which he identifies correctly, can be given a precise mathematical justification. We also gave (for each order in the perturbation expansion) an estimate of the rate at which the contribution of the other diagrams vanishes as t becomes asymptotically large.

We should emphasize here that the non-vanishing of the cumulative effects (as $t \rightarrow \infty$) of the weak interaction is linked in an essential manner to the extensive properties (i.e. lattice-translation invariance \mathbb{Z}^3) of the model. One can indeed verify that *neither* these cumulative effects, *nor* the van Hove diagonal singularity occur unless not only the lattice itself is infinite, but also the impurities are randomly distributed with a finite density over the whole lattice ($M \rightarrow \mathbb{Z}^3$).

Specifically for finite M (or even if the limits occurring in Proposition 2 are taken in the reverse order) one obtains

$$\left(\lim_{M \rightarrow \mathbb{Z}^3} \right) \lim_{\substack{t \rightarrow \infty \\ \lambda^2 t = \tau}} \langle (\varphi, U_{-t}^0 U_t^M \psi) \rangle^M = (\varphi, \psi).$$

This actually is easily seen from an argument, familiar in scattering theory, where the following relation is exploited:

$$\|(U_{-t}^0 U_t^M - I) \varphi\| \leq \lambda \int_0^{\tau/\lambda^2} \|V^M U_s^0 \varphi\| ds.$$

Since here V^M (with M finite) is a finite-rank operator, the integral in the right-hand side is convergent as $\lambda \rightarrow 0$ for a dense set of φ 's in \mathcal{H} [3]. Consequently $U_{-t}^0 U_t^M$ converges strongly to I in the van Hove limit ($t \rightarrow \infty$, $\tau = \lambda^2 t$ fixed), so that no dissipative effect could occur in this case. This is to be brought up together with the fact that, for finite M , V^M does not exhibit any 'diagonal singularity', as can be checked by going through the proof of Lemma 2.1 for this case. The above remark is meant to sustain van Hove's emphasis on the fact that the structural difference between scattering theory and the theory of dissipative phenomena in statistical mechanics has for its origin a difference in the extensive properties of the interaction.

As for the justification of the θ -representation to express these special properties of the interaction, we cannot refrain from quoting van Hove verbatim: 'The special significance of the θ -representation for the many-particle systems of quantum statistics must be attributed to a fact, easily verified on all actual examples, to know: the simple relation of this representation to the physical quantities of greatest interest in irreversible processes.' Specifically the θ -representation is uniquely determined as the spectral representation of the one-particle, lattice-translation invariant observables. H_0 then appears in the theory, not as a result of an arbitrary separation of H^M into $H_0 + \lambda V^M$, but rather as the diagonal part of H^M in this representation. In this sense, a perturbative scheme for this problem appears in a natural manner.

Similarly, the use of the interaction picture (see in particular Section 3) is justified by the fact that one is interested in the time evolution of the expectation values for a particular class of observables, in a particular class of states, which are operationally defined in such a manner that they turn out to be invariant under the free evolution.

We might also remark that the infinite-volume limit having been taken, once and for all, at an early stage of our analysis, we did not have to worry over the fact that certain quantities vary slowly (or are smooth enough) over intervals large against the separation of the energy levels of the unperturbed Hamiltonian: in the limit in which our analysis is conducted H_0 has a truly continuous spectrum.

Finally, we should comment on the occurrence of $\delta(\omega(\theta') - \omega(\theta))$ in our results, and in particular in the master equation obtained in Section 3. It implies that each energy shell evolves independently of the others. In addition, the positivity of the covariance function $g(\theta)$ implies that the master equation, when restricted to an energy shell, admits a unique stationary solution $\rho(\theta) = \rho(\omega(\theta))$ which is a universal attractor. Physically, this means that, in the proper time-scale in which the time evolution is governed by this master equation, $\rho_t(\theta)$ approaches the microcanonical distribution. The occurrence of the microcanonical, rather than the canonical, distribution is of course to be understood from the fact that in our model the impurities are taken to be recoilless, so that, in the limits considered, the unperturbed energy is conserved.

If instead an appropriate quantum Bose bath, at the natural temperature β , were to be introduced the canonical distribution would indeed result. Specifically, one could take [4]

$$\tilde{H}_0 = \int d\theta \omega(\theta) a^*(\theta) a(\theta) + \int d\theta \varepsilon(\theta) b^*(\theta) b(\theta)$$

with

$$\omega(\theta) = \theta^2, \quad \varepsilon(\theta) = (m^2 + \theta^2)^{1/2} - c$$

and

$$\tilde{V} = \iint d\theta d\theta' (v(\theta, \theta') a^*(\theta) b(\theta - \theta') a(\theta') + \text{h.c.})$$

with

$$|v(\theta, \theta')| = |v(\theta', \theta)|,$$

where the a^* (resp. b^*) are the creation and annihilation operators for a Fermi (resp. Bose) field. In this model the Gaussian average is replaced by the thermal average over the system formed by the b -particles, the latter being considered as the system of interest. One can then show [4] by a slight extension of Davies' analysis [5] that the kernel of the master equation becomes, for this model,

$$K(\theta, \theta') = 2\pi |v(\theta, \theta')|^2 (\exp(\beta[\omega(\theta) - \omega(\theta')]) - 1)^{-1} \\ \cdot [\delta(\omega(\theta') - \omega(\theta) + \varepsilon(\theta' - \theta)) - \delta(\omega(\theta') - \omega(\theta) - \varepsilon(\theta' - \theta))]$$

which satisfies the detailed balancing condition

$$K(\theta, \theta') \exp(-\beta\omega(\theta')) = K(\theta', \theta) \exp(-\beta\omega(\theta)).$$

This relation implies that the canonical rather than the microcanonical distribution is the fixed point of the master equation, thus confirming our remark on the cause of the approach to the microcanonical distribution in our model.

From the point of view of the techniques used, we might point out that our analysis could have been cast in the framework of generalized master equations. In this language, Sections 1 and 2 show rigorously that the memory effects vanish in the $\lambda^2 t$ limit and that the Born approximation becomes exact in this limit. There are two differences with the recent works [5, 6] of Davies. First, in our model the spectrum of H_0 is continuous, whereas Davies was concerned with the derivation of Pauli equations for a discrete collection of atomic (or spin) energy levels. Second, and more importantly, the relaxation of systems coupled with thermal baths is linked to a sufficiently fast decrease in time of the correlation functions relative to the bath. These decay properties originate in the nature of the energy spectrum $\varepsilon(\theta)$ of the bath. On the other hand, our system being isolated, the needed decay properties are drawn here from the dispersion law $\omega(\theta)$ of the particles of interest themselves. In both cases, more work is needed to accommodate a phonon-type dispersion law behaving like $c|\theta|$ for small θ 's.

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References

- [1] L. VAN HOVE, *Physica* 21, 517 (1955); see also *Physica* 23, 441 (1957).
- [2] D. RUELLE, *Statistical Mechanics* (Benjamin, New York 1969).
- [3] T. KATO, *Perturbation Theory for Linear Operators* (Springer 1966).
- [4] K. HEPP, private communication.
- [5] E. B. DAVIES, *Markovian master equations*, *Comm. Math. Phys.* 39, 91 (1974).
- [6] E. B. DAVIES, *Comm. Math. Phys.* 27, 309 (1972).