On the van Hove weak-coupling limit for impurity scattering of a quantum particle on a lattice

1996 J. Phys. A: Math. Gen. 29 2553

(http://iopscience.iop.org/0305-4470/29/10/031)

J. Phys. A: Math. Gen. **29** (1996) 2553–2565. Printed in the UK

On the van Hove weak-coupling limit for impurity scattering of a quantum particle on a lattice

Christian Maes† and Wolfgang Spitzer‡

Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium

Received 21 December 1995

Abstract. We consider the problem of quantum impurity scattering for a particle on a lattice via a non-perturbative approach. We calculate the weak-coupling limit in the case of a directed lattice (tree) and we show what problems arise in the more general case due to recurrence effects. Our methods relate the problem to that of a random walk in a random environment.

1. Introduction

An important problem in solid-state physics and in transport theory in general is to understand how the motion of particles is affected by the presence of a random environment. For example, in a real solid, impurity scattering of the conduction electrons is of prime importance in the conductivity properties at low temperatures.

A well known mathematical model is that of a random walk in a random environment or scenery. There we can imagine a classical particle hopping on a lattice while interacting with randomly placed impurities. A central theme is the derivation of diffusive behaviour for the appropriately rescaled time evolution. At the end of section 6 we will come back to a possible relation between our work here and some no-go theorem that recently appeared for that classical problem.

An appropriate model for the motion of a quantum particle is the Anderson model. The time evolution is now generated by the random Schrödinger operator $H^\lambda = -\Delta + \lambda V$. Δ is the finite-difference (discrete) Laplacian and V the random potential. The strength of the potential is parametrized by $\lambda > 0$.

In this paper we study the so-called weak-coupling limit for the pair $(-\Delta, H^\lambda)$. In that limit, $\lambda \downarrow 0$ while the product $t\lambda^2$ (t is the time variable) remains constant. This procedure has also become known as the van Hove limit, see [Hov].

The problem of this weak-coupling limit has been taken up by many but has invariantly been based on Dyson-expansion techniques. The most successful applications are, however, restricted to the continuum case with Δ being the Laplacian on $\mathbb{R}^d$. The most complete discussions are in [HLW] and [Lan]. Some of these techniques appeared already in the work of Spohn [Spo] and Martin and Emch [ME]. The models studied by [ME] and Hugenholtz [Hug] are lattice models and contain some gaps in the proofs. The question is whether this can be repaired in order to get similar results as in the continuum case.

† Onderzoeksleider NFWO (e-mail address: Christian.Maes@fys.kuleuven.ac.be).

‡ On leave from: Vienna, Boltzmanng. 5, A-1090, Austria (e-mail address: Spitzer@pap.univie.ac.at).

0305-4470/96/102553+13$19.50

In this paper we take a different route. Our approach is non-perturbative and we obtain a correspondence between the original quantum problem and a related problem of a random walk in a random environment. This, as often, goes via some kind of functional integration formula which, however, does not seem to be very well known for the model at hand. Such a path integral method applied to coupled systems as the one we study here first appeared in the work of [FV]. This procedure is therefore sometimes called the Feynman–Vernon method.

After the presentation of the model in the next section, we give a self-contained proof of our basic starting point (in [C] it is called the Molchanov formula) in section 3.

Section 4 is devoted to the study of the weak-coupling limit for a particle hopping on a tree. We explicitly calculate the limiting motion for various choices of the distribution of the random potential V. The problem of recurrence effects is studied in the last sections. We show what can go wrong and what this implies for motion on a regular lattice.

2. The model

Let us consider a directed graph $\mathcal{D}$ with vertex set $\mathcal{L}$. Each vertex has a finite (uniformly bounded) and non-zero number of neighbours (adjacent vertices). For all the edges that leave vertex $x \in \mathcal{L}$, a fraction $\Delta_{xy} \geqslant 0$ leads to the neighbour $y \in \mathcal{L}$ and a fraction $1 + \Delta_{xx} \geqslant 0$ leads to itself. With each vertex $x \in \mathcal{L}$ there is associated a random variable $V(x)$ (taking values in $\mathbb{R}$) with joint distribution Q. Expectation with respect to this random field is denoted by $\mathbf{E}_V$. Conditions on the distribution Q will be stated later but we always assume that $\mathbf{E}_V(V(x)) = 0, \mathbf{E}_V(V(x)^2) =: V^2 < \infty$. We will consider bounded complex-valued functions $f : \mathcal{L} \to \mathbb{C}$ and define

$$\Delta f(x) = \sum_{y\in\mathcal{L}} \Delta_{xy} f(y). \tag{2.1}$$

Δ is the usual lattice Laplacian in the case $\mathcal{L} = \mathbb{Z}^d$, $\Delta_{xy} = 1/2d$ for nearest neighbours and $\Delta_{xx} = -1$.

The random Schrödinger operator H^λ is then given by

$$H^\lambda f(x) = -\Delta f(x) + \lambda V(x) f(x) \tag{2.2}$$

with $\lambda > 0$. H^λ is a self-adjoint operator on $l^2(\mathcal{L})$ if $\mathcal{L} = \mathbb{Z}^d$. We are then dealing with the widely studied Anderson model on $\mathbb{Z}^d$. We are interested in the dynamical (real-time) evolution generated by H^λ when we rescale the time by λ^2 and let $\lambda \downarrow 0$. In other words, our problem is to analyse the limit $\lambda \downarrow 0, t \uparrow \infty$ such that $t\lambda^2 = t_0$ of

$$\alpha_t^\lambda f = \mathrm{e}^{-\mathrm{i}tH^\lambda} \mathrm{e}^{-\mathrm{i}\Delta t} f \tag{2.3}$$

for functions f on $\mathcal{L}$ describing the initial state of the particle. This corresponds to a scattering problem in a random environment since α_t^λ contains the random potential V. The limit is meant in the weak sense, i.e. we are interested in

$$\lim_{\substack{\lambda^2 t = t_0 \\ \lambda\downarrow 0}} \mathbf{E}_V(\alpha_t^\lambda f). \tag{2.4}$$

In other cases (where the graph $\mathcal{D}$ is really directed) H^λ will not be self-adjoint but we will take advantage of our more general set-up in section 4 to prepare the case $\mathcal{L} = \mathbb{Z}^d$.

Note that the potential V can be considered as the reservoir in the traditional approach to the weak-coupling limit but we have assumed this reservoir being relaxed and thus not evolving in time.

The main goal of this paper is to show how one can relate this problem to a classical random walk in a random scenery. With this new approach we get explicit results for the limiting behaviour for certain choices of the free evolution Δ on $\mathcal{L}$ and we identify situations in which the limit does in fact not exist.

3. A Feynman-type formula

Our approach is based on a Feynman-type formula for quantum evolutions on discrete spaces which seems to be little known. In [C] it is called the Molchanov formula. Our presentation is self-contained, but we do not give the most direct proof (a shorter, more direct proof can be found in [C]). We do this to be able to introduce some calculations and formulae we need in the following sections.

Proposition 1. Let $\mathbf{E}_{x_0=x}$ denote the expectation with respect to the continuous time random walk $x_s, s \geqslant 0$, on $\mathcal{D}$ generated by Δ. Let $N(t)$ be the Poisson process giving the number of jumps of the walk in the time interval $[0, t)$. Then, for all bounded complex-valued functions f, for all bounded real-valued functions V, and for all $x \in \mathcal{L}$

$$\mathrm{e}^{-\mathrm{i}(-\Delta+V)t} f(x) = \mathrm{e}^{(1-\mathrm{i})t}\mathbf{E}_{x_0=x}\left[\mathrm{i}^{N(t)} f(x_t) \exp\left(-\mathrm{i}\int_0^t V(x_s)\,\mathrm{d}s\right)\right]. \tag{3.1}$$

Proof. Consider the right-hand side of (3.1). This is an expectation for a continuous time random walk x_s but we can replace this by a similar expectation over the underlying discrete time random walk $x(n), x(0) = x, n = 0, 1, \ldots,$ if we think of $x(n)$ as the position of the continuous time random walker after the n-th jump. This discrete time random walk $x(n)$ on $\mathcal{D}$ is given by the transition probabilities

$$\mathrm{Prob}[x(n) = y | x(n-1) = z] = \Delta_{zy} \qquad z \neq y$$

$$\mathrm{Prob}[x(n) = y | x(n-1) = y] = 1 + \Delta_{yy}.$$

All we have to do is to integrate out the waiting times for the continuous time random walk. To do this, let us insert the identity $1 = \sum_{k\geqslant 0} I[N(t) = k]$ into the expectation in (3.1), where $I[N(t) = k]$ is the indicator function of having exactly k jumps in time $[0, t)$. Note that if $N(t) = k$, then

$$\int_0^t V(x_s)\,\mathrm{d}s = \sum_{n=0}^{k-1} V(x(n))\tau_n + V(x(k))\left(t - \sum_{n=0}^{k-1}\tau_n\right)$$

where $\tau_n, n = 0, \ldots, k$ is a family of independent and identically exponentially distributed random variables with mean 1 (these are the waiting times) conditioned on (the fact that $N(t) = k$ if and only if)

$$0 \leqslant t - \sum_{n=0}^{k-1}\tau_n < \tau_k.$$

We therefore have

$$\mathbf{E}_{x_0=x}\left\{f(x_t)\exp\left(-\mathrm{i}\int_0^t V(x_s)\,\mathrm{d}s\right)I[N(t) = k]\right\}$$

$$= \mathbf{E}_{x(0)=x}\left\{f(x(k))\int_0^\infty \mathrm{d}\tau_0\cdots\int_0^\infty \mathrm{d}\tau_k\ I\left[0 \leqslant t - \sum_{n=0}^{k-1}\tau_n < \tau_k\right]\mathrm{e}^{-\tau_0-\tau_1-\cdots-\tau_k}\right.$$

$$\times \exp\left(-\mathrm{i}\left[\sum_{n=0}^{k-1} V(x(n))\tau_n + V(x(k))\left(t - \sum_{n=0}^{k-1}\tau_n\right)\right]\right\}$$

$$= \mathrm{e}^{-t}\mathbf{E}_{x(0)=x}\left\{f(x(k))\tilde{F}_k(t,V)\right\}$$

where

$$\tilde{F}_k(t,V) = \int_0^\infty \mathrm{d}\tau_0 \cdots \int_0^\infty \mathrm{d}\tau_{k-1}\; I\left[\sum_{n=0}^{k-1}\tau_n \leqslant t\right]$$

$$\times \exp\left(-\mathrm{i}\left[\sum_{n=0}^{k-1} V(x(n))\tau_n + V(x(k))\left(t - \sum_{n=0}^{k-1}\tau_n\right)\right]\right)$$

for $k \geqslant 1$, and $\tilde{F}_0(t,V) = \mathrm{e}^{-\mathrm{i}V(x)t}$. Now, note that

$$\tilde{F}_k(t,V) = \mathcal{L}^{-1}F_k(\cdot,V)(t)$$

is the inverse Laplace transform of

$$F_k(p,V) = \prod_{n=0}^{k}\int_0^\infty \mathrm{d}\tau\; \mathrm{e}^{-p\tau}\mathrm{e}^{-\mathrm{i}V(x(n))\tau}$$

$$= \prod_{n=0}^{k}\frac{1}{p + \mathrm{i}V(x(n))} \tag{3.2}$$

for $p \in \mathbb{C}\setminus\mathbb{R}^-$. Hence the right-hand side of equation (3.1) equals

$$\mathrm{e}^{-\mathrm{i}t}\mathcal{L}^{-1}\left[\sum_{k\geqslant 0}\mathrm{i}^k\mathbf{E}_{x(0)=x}\left\{f(x(k))\prod_{n=0}^{k}\frac{1}{p+\mathrm{i}V(x(n))}\right\}\right](t). \tag{3.3}$$

Now, using the Markov property of the random walk the expectation $\mathbf{E}_{x(0)=x}\{\cdot\}$ equals

$$\frac{1}{p+\mathrm{i}V(x)}\cdot\mathbf{E}_{x(0)=x}\left\{\frac{1}{p+\mathrm{i}V(x(1))}\cdot\mathbf{E}_{y(0)=x(1)}\left[f(y(k-1))\prod_{n=0}^{k-1}\frac{1}{p+\mathrm{i}V(y(n))}\right]\right\}$$

where $y(n)$ is the (discrete) random walk starting at $y(0) = x(1)$. Iterating this procedure we get

$$\text{equation (3.3)} = \mathrm{e}^{-\mathrm{i}t}\mathcal{L}^{-1}\left\{(p+\mathrm{i}V)^{-1}\sum_{k\geqslant 0}\left[\mathrm{i}(\Delta+1)(p+\mathrm{i}V)^{-1}\right]^k\right\}(t)f(x)$$

and hence we conclude that the right-hand side of (3.1) equals

$$\mathrm{e}^{-\mathrm{i}t}\mathcal{L}^{-1}\left\{(p+\mathrm{i}V)^{-1}\frac{1}{1-\mathrm{i}(\Delta+1)(p+\mathrm{i}V)^{-1})}\right\}(t)f(x)$$

$$= \mathrm{e}^{-\mathrm{i}t}\mathcal{L}^{-1}\left\{\frac{1}{p+\mathrm{i}V-\mathrm{i}(\Delta+1)}\right\}(t)f(x)$$

$$= \mathrm{e}^{-\mathrm{i}(-\Delta+V)t}f(x).$$

$\square$

4. The case without loops

We start the evaluation of the limit $\lambda \downarrow 0, \lambda^2 t = t_0$ (constant) for the case where $\mathcal{D}$ is a directed tree. This implies that for all paths $x(n)$, starting at $x(0) = x$ the distance (number of jumps) $d(x(n), x) = n$. Moreover we restrict ourselves to the case where for all paths $V(x(n)) = V_n$ is a binary symmetric Markov chain. That is, $V_n = \pm V$ with transition probabilities

$$\mathrm{Prob}[V_n = +V | V_{n-1} = +V] = \mathrm{Prob}[V_n = -V | V_{n-1} = -V] \equiv \gamma$$

with $\gamma \in [0, 1]$. The simplest example is that of a Bernoulli random field $(V(x), x \in \mathcal{L}), V(x) = \pm V$ with equal probability on $\mathcal{D} =$ directed Bethe lattice, corresponding to $\gamma = \frac{1}{2}$. The case $\gamma \neq \frac{1}{2}$ is obtained by taking the $(V(x), x \in \mathcal{B})_{\mathcal{B}}$ independent and identically distributed Markov chains for each of the branches $\mathcal{B}$ of the tree starting from a common vertex.

Theorem 4.1. Suppose that for all $x \in \mathcal{L}$ and for all paths $x(n)$ with $x(0) = x$ on the directed tree $\mathcal{D}$, $V(x(n)) = V_n$ is a binary symmetric Markov chain with parameter γ $(\gamma \neq 1)$ as above. Then

$$\lim_{\lambda\downarrow 0} \mathbf{E}_V(\alpha_t^\lambda f) = \exp\left(\mathrm{i}\frac{t_0}{2(1-\gamma)}\frac{V^2}{\Delta+1}\right) f \tag{4.1}$$

uniformly on compacts ($t_0 \in K =$ compact), and pointwise for bounded functions $f : \mathcal{L} \to \mathbb{C}$.

Remark. $(\Delta+1)^{-1} f(x) = f(y)$, where y is the uniquely determined vertex for which there is an arrow from y to x. In particular, $\Delta_{xx} = -1$. Therefore, $\|(\Delta+1)^{-1}\|_\infty = 1$.

Proof. We must take the expectation $\mathbf{E}_V$ of equation (3.3). The important thing to note is that under the hypothesis of the theorem, the expectation over the random walk and the expectation over the random field factorizes. This means that (with $f_t = \mathrm{e}^{-\mathrm{i}\Delta t} f$)

$$\begin{aligned}
\mathbf{E}_V \mathbf{E}_{x(0)=x}\left\{f_t(x(k))\tilde{F}_k(t, \lambda V)\right\} &= \mathcal{L}^{-1}\left(\mathbf{E}_V \mathbf{E}_{x(0)=x}\left\{f_t(x(k))\prod_{n=0}^{k}\frac{1}{p+\mathrm{i}\lambda V(x(n))}\right\}\right)(t) \\
&= \mathcal{L}^{-1}\left(\mathbf{E}_{x(0)=x}\left\{f_t(x(k))\mathbf{E}_V\left[\prod_{n=0}^{k}\frac{1}{p+\mathrm{i}\lambda V(x(n))}\right]\right\}\right)(t) \\
&= (\Delta+1)^k f_t(x)\mathcal{L}^{-1}\left(\mathbf{E}_V\left[\prod_{n=0}^{k}\frac{1}{p+\mathrm{i}\lambda V_n}\right]\right)(t).
\end{aligned} \tag{4.2}$$

We will rewrite the expectation value w.r.t. V as

$$\begin{aligned}
\mathbf{E}_V\left[\prod_{n=0}^{k}\frac{1}{p+\mathrm{i}\lambda V_n}\right] &= \frac{1}{2}\,\mathrm{tr}\left[\begin{pmatrix} \frac{\gamma}{p+\mathrm{i}\lambda V} & \frac{1-\gamma}{p-\mathrm{i}\lambda V} \\ \frac{1-\gamma}{p+\mathrm{i}\lambda V} & \frac{\gamma}{p-\mathrm{i}\lambda V}\end{pmatrix}^k \cdot \begin{pmatrix} \frac{1}{p+\mathrm{i}\lambda V} & \frac{1}{p-\mathrm{i}\lambda V} \\ \frac{1}{p+\mathrm{i}\lambda V} & \frac{1}{p-\mathrm{i}\lambda V}\end{pmatrix}\right] \\
&= \tfrac{1}{2}\,\mathrm{tr}[M^k M'].
\end{aligned}$$

Now we use the fact that (3.3) = (3.1) and get

$$\mathbf{E}_V(\alpha_t^\lambda f(x)) = \frac{1}{2}\mathrm{e}^{-\mathrm{i}t}\mathcal{L}^{-1}\left[\sum_{k\geqslant 0}(\mathrm{i}(\Delta+1))^k f_t(x)\,\mathrm{tr}(M^k M')\right](t).$$

Note that $\Delta + 1$ is a bounded operator on $L^\infty(\mathcal{L})$. The last expression equals

$$\frac{1}{2}\mathrm{e}^{-\mathrm{i}(\Delta+1)t}\frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\mathrm{d}p\ \mathrm{e}^{pt}\ \mathrm{tr}[(1-\mathrm{i}(\Delta+1)M)^{-1}M']f(x)$$

where in order to get a summable series we have shifted the line of integration parallel to the imaginary axis. Now

$$\mathrm{tr}[(1-\mathrm{i}(\Delta+1)M)^{-1}M'] = 2\,\frac{p-\mathrm{i}(\Delta+1)(2\gamma-1)}{(p-A_+)(p-A_-)}$$

where

$$A_\pm = \mathrm{i}(\Delta+1)\left\{\gamma \pm \sqrt{(1-\gamma)^2 + (\Delta+1)^{-2}\lambda^2V^2}\right\}.$$

Since $(\Delta+1)^{-1}$ is a bounded operator the square root is well defined for small λ by its series expansion in the point $(1-\gamma)^2$. By using the residue calculus (no problems arise because the operators $A_\pm$ are bounded) for the inverse Laplace transform we get

$$\mathrm{e}^{-\mathrm{i}(\Delta+1)t}\left[(1+\mathrm{O}(\lambda))\mathrm{e}^{tA_+} + \mathrm{O}(\lambda)\mathrm{e}^{tA_-}\right]f(x)$$
$$= \big(1+\mathrm{O}(\lambda)\big)\exp\left(\mathrm{i}t\left[\frac{\lambda^2V^2}{2(1-\gamma)(\Delta+1)} + \mathrm{O}(\lambda^3)\right]\right)f(x) + \mathrm{O}(\lambda).$$

Rescaling time as $t = t_0\lambda^{-2}$ we finally get the result (4.1). □

Remarks. (i) If we take a general random field $(V(x), x \in \mathcal{L})$ of independent and identically distributed random variables with $\mathbf{E}_V(V) = 0$, $\mathbf{E}_V(V^2) < \infty$, then one can show that the same result (4.1) with $\gamma = \frac{1}{2}$ holds.

(ii) It is obvious how to generalize to the case where $\mathbf{E}_V(V(x)) = \lambda m \neq 0$. In that case one must simply multiply the limit in (4.1) by $\mathrm{e}^{-\mathrm{i}mt_0}$.

(iii) The limit does not exist when $\gamma = 1$.

5. Finite systems

5.1. Finite Laplacian

Now we consider a cube $\mathcal{L} \subset \mathbb{Z}^3$ centred at the origin containing N^3 sites, and Δ (generating the free time evolution on $\mathcal{L}$) being the finite volume Laplacian with periodic boundary conditions on $\mathcal{L}$. The reciprocal lattice $\mathcal{L}^*$ (first Brillouin zone) contains the points $\theta \in \{0, 2\pi(1/N), \ldots, 2\pi(N-1)/N\}^3$ and if $\theta, \theta' \in \mathcal{L}^*$, then

$$\sum_{x,y\in\mathcal{L}} \mathrm{e}^{\mathrm{i}x\theta}\mathrm{e}^{-\mathrm{i}y\theta'}\mathbf{E}_V(V(x)V(y)) = N^3\delta_{\theta,\theta'}V^2$$

if the $\{V(x)\}$ are independent. This property is called van Hove's diagonal singularity condition. If we would then take the control of the Dyson series (exchange of limits, see lemma 2.2 of [ME]) for granted and apply the proof presented in [ME], we would get a well-defined weak-coupling limit for $\mathbf{E}_V(f, \alpha_t^\lambda g)$ where f and g are functions on $\mathcal{L}$.

Let us, however, inspect what finite volume computations give. Consider finite graphs $(\mathcal{D}, \Delta)$ of n vertices with Δ symmetric (see the beginning of section 2). Since n is finite, we take realizations of the potential V for which $\sum_{x\in\mathcal{L}} V(x) = 0$.

Let $m_i(\lambda), 1 = 1, \ldots, n$ be the eigenvalues of the matrix $H^\lambda = -\Delta + \lambda V$. They converge to $m_i(0) = m_i$ (the eigenvalues of $-\Delta$) as $\lambda \to 0$. In the same way, the scalar product $\langle m_j(\lambda)|m_i\rangle$ goes to $\delta_{i,j}$ $(i, j = 1, \ldots, n)$ as $\lambda \to 0$ where the $\{|m_j(\lambda)\rangle\}$ are a basis of orthonormal eigenvectors of H^λ. We thus have that

$$\langle m_i|\mathrm{e}^{-\mathrm{i}tH^\lambda}\mathrm{e}^{-\mathrm{i}t\Delta}|m_j\rangle \to 0 \qquad \text{for } i \neq j, \lambda \to 0$$

and

$$\langle m_i|\mathrm{e}^{-\mathrm{i}tH^\lambda}\mathrm{e}^{-\mathrm{i}t\Delta}|m_i\rangle = \sum_j |\langle m_j(\lambda)|m_i\rangle|^2 \mathrm{e}^{-\mathrm{i}t(m_j(\lambda)-m_i)}$$

$$= \mathrm{e}^{-\mathrm{i}t(m_i(\lambda)-m_i)} + \mathrm{O}(\lambda).$$

But $m_i(\lambda) - m_i = \mathrm{O}(\lambda)$ in general (except when $n = 2$). This means that the weak-coupling limit (where time is rescaled as $\lambda^2 t = t_0$) cannot exist here. This remains true when we average over the potential V (say with independent identically distributed random variables $V(x) = 0, \pm 1$) conditioned on $\sum_{x\in\mathcal{L}} V(x) = 0$.

Confronting this with the assumed control of the Dyson series (above) we come to the conclusion that we cannot hope for success via a (perturbative) Dyson-series approach in the lattice case. The infinite-volume version of this argument should be based on equation (6.7) but as we saw here, the same difficulty is already apparent at finite volumes.

5.2. Finite disorder

For any graph with a zero density of impurities the weak-coupling limit gives the identity. This means that if we take an infinite graph but put $V(x) = 0$ except on a finite number on vertices, then $\lim_{\lambda\downarrow 0} \alpha_t^\lambda f = f$. This was shown in [ME] and we just want to mention here how this follows from our representation (3.1). Suppose that $|V(x)| \leqslant V$ and $V(x) = 0$ for $x \notin M$ with M a finite region in $\mathbb{Z}^3$. Then

$$\left| \int_0^t V(x_s)\,\mathrm{d}s \right| \leqslant V\,T(t, M)$$

where $T(t, M)$ is the total time spent by the random walk in the region M up to time t. But $\mathbf{E}[T^2(t, M)] \leqslant \mathbf{E}[T^2(\infty, M)] < \infty$ so that $\lambda \int_0^t V(x_s)\,\mathrm{d}s$ converges to zero in distribution as $\lambda \sim t^{-2}$ goes to 0.

6. The general case

6.1. Some heuristics

The main hope in our non-perturbative approach to this weak-coupling limit lies in the representation of the quantum evolution via a classical stochastic process (random walk in a (complex) random environment). This relation introduces a body of insights (results and intuition) which is just not available on the operator level of the problem. An illustration of that can be found in the understanding why one would like to scale the random field by λ, while rescaling time as $t = t_0\lambda^{-2}$. What happens is that, as $t \to \infty$, the integral in the Molchanov formula (3.1) behaves like

$$\lambda \int_0^t V(x_s)\,\mathrm{d}s \simeq \lambda\sqrt{t} \cdot \xi = \sqrt{t_0} \cdot \xi \tag{6.1}$$

with ξ a Gaussian random variable as follows from a central limit theorem for the random variables $V(x_s)$ with distribution induced from that of the random walk x_s and of the random field $V(x)$.

Here is a heuristic way of deriving theorem 4.1 based on this observation. Suppose that we condition on the number of jumps $N(t) = k$ (this has probability $e^{-t} t^k/k!$) in our expectation $\mathbf{E}_{x_0=x}$ of (3.1). We further assume that the waiting times in $[0, t)$ are simply equal to $\tau = t/(k+1)$. Then, approximately, we get that $\mathbf{E}_V(\alpha_t^\lambda f)$ equals (with $f_t = e^{-i\Delta t}$)

$$e^{-it}\mathbf{E}_V\mathbf{E}_{x_0=x}\left\{i^{N(t)} f_t(x_t)\exp\left(-i\lambda\int_0^t V(x_s)\,ds\right)\right\}$$

$$\simeq e^{-it}\sum_{k\geqslant 0}\frac{(it(\Delta+1))^k}{k!} f_t(x)\mathbf{E}_V\left(\exp\left(-i\lambda\frac{t}{k+1}\sum_{n=0}^{k} V_n\right)\right).$$

Assuming central-limit behaviour, we can estimate this last expression by

$$e^{-it(\Delta+1)}\cdot\sum_{k\geqslant 0}\frac{(it(\Delta+1))^k}{k!} f(x)\exp\left(-\frac{1}{2}\frac{t^2}{k+1}\lambda^2\chi_V\right)$$

with $\chi_V = \sum_{n\geqslant 0}\mathbf{E}_V[V_0V_n] = V^2/(2(1-\gamma))$. Now, it is not so difficult to convince oneself that

$$\lim_{\lambda\downarrow 0} e^{-iy\lambda^{-2}}\sum_{k\geqslant 0}\frac{(iy\lambda^{-2})^k}{k!} g(k\lambda^2) = g(iy) \tag{6.2}$$

for a class of sufficiently regular functions g. Applying this to the function $f(r) = e^{-\frac{1}{2}\chi_V/r}$ we get indeed the limit (4.1) of theorem 4.1 (except for the factor $\frac{1}{2}$). It is obvious that there must be huge cancellations in (6.2) for the limit to exist. For example, if we replace $g(k\lambda^2)$ by a more general dependence, say $\hat{g}(k, \lambda^2)$ then the limit (6.2) fails to exist in general. Now, if we trust that approximating the waiting times in the calculation of (3.1) does perhaps not give exactly the correct limit but at least gives some hint of what the correct limit may be, then we end up exactly with a calculation as in (6.2) but with $g(k\lambda^2)$ replaced by $\hat{g}(k, \lambda^2)$. And hence the existence of the weak-coupling limit seems very doubtful.

The arguments above also give support to the conclusion that the quantum weak-coupling limit, if it exists, should be independent of the details of the random field V (and one has the same universality as in the central-limit theorem).

6.2. One-loop pathologies

We illustrate here via a simple example what can go wrong in the weak-coupling limit because of recurrence effects in the associated random walk.

Take a linear chain $\mathcal{L} = \mathbb{Z}$ for which we draw for each $x \in \mathbb{Z}$ an arrow from x to $x+1$ and a loop from $x = 0$ to $x = 0$. This means that $\Delta_{xy} = 1$ if $y = x+1, x \neq 0$, $\Delta_{xx} = -1$ if $x \neq 0$, $-\Delta_{00} = \Delta_{01} = \frac{1}{2}$ and all the other matrix elements are zero. The operator Δ is now

$$\Delta f(x) = \begin{cases} \frac{1}{2}[f(1) - f(0)] & x = 0 \\ f(x+1) - f(x) & x \neq 0 \end{cases}$$

with σ_+ being the right shift on $\mathbb{Z}$. This means that for walks starting at $x = 0$, there are the following possibilities which can be realized: if $k \geqslant 1$ is the number of steps in the walk, then

$$x(0), x(1), \ldots, x(k) = \begin{cases} 0, 1, \ldots, k & \text{with probability } \frac{1}{2} \\ 0, 0, 1, \ldots, k-1 & \text{with probability } (\frac{1}{2})^2 \\ 0, 0, 0, \ldots, k-2 & \text{with probability } (\frac{1}{2})^3 \\ \qquad \vdots & \\ 0, 0, \ldots, 0, 1 & \text{with probability } (\frac{1}{2})^k \\ 0, 0, \ldots, 0 & \text{with probability } (\frac{1}{2})^k. \end{cases}$$

Next we calculate the expectation appearing in (3.3):

$$\sum_{k\geqslant 0} \mathrm{i}^k \mathbf{E}_{x(0)=x} \left\{ f(x(k)) \prod_{n=0}^{k} \frac{1}{p + \mathrm{i}\lambda V(x(n))} \right\}$$

$$= \sum_{k=1}^{\infty} \mathrm{i}^k \sum_{l=0}^{k-1} f_t(k-l) \left(\frac{1}{2}\right)^{l+1} \mathbf{E}_V \left[\left(\frac{1}{p + \mathrm{i}\lambda V} \right)^{l+1} \right] \prod_{n=0}^{k-1} \mathbf{E}_V \left(\frac{1}{p + \mathrm{i}\lambda V(n)} \right)$$

$$+ \sum_{k=0}^{\infty} \mathrm{i}^k \left(\frac{1}{2}\right)^k f_t(0) \mathbf{E}_V \left[\left(\frac{1}{p + \mathrm{i}\lambda V(0)} \right)^{k+1} \right] \tag{6.3}$$

with $f_t = \mathrm{e}^{-\mathrm{i}t\Delta} f$. We show in the appendix that for a constant function $f \equiv a$ equation (6.3) is equal to

$$\frac{1}{2} a \left[\frac{\mathrm{i}p}{p^2 - \mathrm{i}p + \lambda^2 V^2} - \mathrm{i} \frac{p \pm \mathrm{i}\lambda V}{p \pm \mathrm{i}\lambda V - 2\mathrm{i}} \right] \frac{p}{(p \pm \mathrm{i}\lambda V)^2} + \frac{1}{2} a \frac{1}{p \pm \mathrm{i}\lambda V - \frac{1}{2}\mathrm{i}}. \tag{6.4}$$

Now, according to equation (3.3) we take the inverse Laplace transform w.r.t. p in the point t and then multiply the whole with $\mathrm{e}^{-\mathrm{i}t}$. By using the residue calculus we find the term $a \exp\big(\mathrm{i}t(\lambda^2 V^2 + \mathrm{O}(\lambda^3))\big)$ stemming from the roots of $p^2 - \mathrm{i}p + \lambda^2 V^2$ plus bounded (in λ) terms which come from the other roots being of the form constant $+\,\mathrm{O}(\lambda)$. Rescaling time as $t = t_0 \lambda^{-2}$ we get convergence of the first term to $a\mathrm{e}^{\mathrm{i}t_0 V^2}$ and oscillating terms like $\exp\big(\mathrm{i}t_0 \lambda^{-1} V\big)$ which do *not* converge in the limit $\lambda \downarrow 0$ and which do not cancel each other because they also appear at different frequencies.

In the convergent term $a\mathrm{e}^{\mathrm{i}t_0 V^2}$ we recognize the result (4.1) of the weak-coupling limit for the case of a tree on $\mathbb{Z}$ with $\gamma = \frac{1}{2}$; $(\Delta + 1)^{-1}$ is equal there to the left shift.

The result for the one-loop example is so to say the result as for the no-loop case plus oscillating non-convergent terms arising from the presence of a single loop at 0.

In the sense of distributions one would always get a limit of $\alpha_t^\lambda f = \mathrm{e}^{-\mathrm{i}H^\lambda t} \mathrm{e}^{-\mathrm{i}\Delta t} f$ because $\alpha_t^\lambda f$ is a bounded function of λ. In the one-loop example this would mean that we simply neglect (or project out all paths with at least one loop) the oscillating terms, because viewed as distributions they tend to 0 as $\lambda \downarrow 0$.

Remark. We can think of this continuous time random walk with the single loop at 0 as a random walk without loops and with exponentially distributed waiting times (as usual) except at the point 0 where we have a geometric distribution of the waiting time.

6.3. The regular-lattice case

Consider finally the problem of the weak-coupling limit on $\mathcal{L} = \mathbb{Z}^d$ ($d \geqslant 3$) with the usual lattice Laplacian. We take the $(V(x), x \in \mathbb{Z}^d)$ to be a random field of independent and identically distributed random variables taking the values $V(x) = \pm 1$. The difference with the analysis of section 4 is of course that now the graph $\mathcal{D}$ contains loops.

In the previous example of section 6.2, we saw how the presence of just one loop (and even when it can be visited only once by the random walker) already has the effect of destroying the weak-coupling limit. We will next argue why for the regular-lattice case we also expect that this limit may not exist.

Consider the functional integral (3.1). It can be viewed as consisting of two parts. There is a first factor $\mathrm{e}^{(1-\mathrm{i})t}\mathrm{i}^{N(t)}$ which has expectation equal to one. Note, however, that the variance

$$\mathrm{e}^{2(1-\mathrm{i})t}\mathbf{E}_{x_0=x}[(-1)^{N(t)}] = \mathrm{e}^{-2\mathrm{i}t}$$

is strongly oscillating as $t \uparrow \infty$. The question is how these oscillations can be cancelled by the second factor. For this second factor we know from [KV] and [MFGW] that

$$\lim_{t\uparrow\infty} \mathbf{E}_V \mathbf{E}_{x_0=x}\left[\exp\left(-\mathrm{i}\sqrt{\frac{t_0}{t}}\int_0^t V(x_s)\,\mathrm{d}s\right)\right] = \mathrm{e}^{-\frac{1}{2}t_0\chi_V}$$

where

$$\begin{aligned}
\chi_V &= \lim_{t\uparrow\infty} \mathbf{E}_V \mathbf{E}_{x_0=x}\left[\frac{1}{t}\int_0^t\int_0^t V(x_s)V(x_{s'})\,\mathrm{d}s\,\mathrm{d}s'\right] \\
&= V^2 \lim_{t\uparrow\infty} \mathbf{E}_{x_0=x}\left[\frac{1}{t}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s'\,\delta_{x_s,x_{s'}}\right] \\
&= V^2 \lim_{t\uparrow\infty} \frac{1}{t}\mathbf{E}_{x_0=x}\left[\sum_{y\in\mathbb{Z}^d} l^2(y,t)\right]
\end{aligned}$$

where $l(y,t) = \int_0^t \delta_{x_s,y}$ is the local time spent by the walk on the point y up to time t. But $\mathbf{E}_{x_0=x}[l^2(y,t)] \leqslant \mathbf{E}_{x_0=x}[l^2(x,t)]$ so that

$$\begin{aligned}
\mathbf{E}_{x_0=x}\left[\sum_{y\in\mathbb{Z}^d} l^2(y,t)\right] &\leqslant \mathbf{E}_{x_0=x}[l^2(x,t)N(t)] \\
&\leqslant \mathbf{E}[N(t)]\mathbf{E}_{x_0=x}[l^2(x,\infty)].
\end{aligned}$$

Hence

$$\chi_V \leqslant V^2\mathbf{E}_{x_0=x}[l^2(x,\infty)] < \infty$$

by the transience of the continous time simple random walk on $\mathbb{Z}^d$, $d \geqslant 3$.

Now because of the presence of loops the expectation in (3.1) does not factorize as a product over the two factors above (this did happen in the directed tree case of section 4). Moreover we must insert the initial wavefunction f. We must therefore consider the expectation of the second factor

$$g(t,k) = \mathbf{E}_V\mathbf{E}_{x_0=x}\left[\mathrm{e}^{-\mathrm{i}\Delta t} f(x_t)\exp\left(-\mathrm{i}\sqrt{\frac{t_0}{t}}\int_0^t V(x_s)\,\mathrm{d}s\right)\middle| N(t) = k\right] \tag{6.5}$$

for a fixed number of jumps $N(t) = k$, and require that the behaviour of the weak-coupling limit be

$$\lim_{\lambda^2 t = t_0, \lambda \downarrow 0} \mathbf{E}_V(\alpha_t^\lambda f) = \lim_{t \uparrow \infty} \mathrm{e}^{-\mathrm{i}t} \sum_{k=0}^{\infty} \frac{(\mathrm{i}t)^k}{k!} g(t,k). \tag{6.6}$$

Clearly there are choices of g for which this last limit makes sense. For example, we can take $g(t,k) = \mathrm{e}^{-\mathrm{i}t} 2^k$ but also $g(t,k) = \int_0^\infty \mathrm{d}p\ h(p)\mathrm{e}^{-pk/t}$ for some $h \in L^1[0,\infty)$ gives a well-defined limit. However, the reader will not have any difficulty in finding functions $g(t,k)$ for which the limit does not exist and in realizing that the behaviour of $g(t,k)$ for *small* k matters very much. This to say that the existence of the limit (6.6) is a very subtle business.

So let us look back at the expression (6.5) for $g(t,k)$. Taking the expectation over the disorder, we have

$$g(t,k) = \mathbf{E}_{x_0 = x}\left[\mathrm{e}^{-\mathrm{i}\Delta t} f(x_t) \exp\left(\frac{V^2}{2}\frac{t_0}{t}\sum_y l^2(y,t)\right)\Bigg| N(t) = k\right].$$

It does not seem unreasonable to expect that when we stop the process when $N(t) = k$, that

$$\sum_y l^2(y,t) \simeq k^{d/2}\left(\frac{t}{k^{d/2}}\right)^2 = \frac{t^2}{k^{d/2}}.$$

It leads us to believe that

$$g(t,k) \simeq \mathrm{e}^{-\mathrm{i}\Delta t}(1+\Delta)^k f(x) \exp\left(-\frac{V^2}{2}\frac{t}{k^{d/2}}\right).$$

The limit (6.6) does not exist for this last choice of $g(t,k)$.

This scepticism can be further substantiated by referring to the results about loop condensation effects in the behaviour of random walks in a random scenery as recently obtained by [KMSS]. Theorem 3 of [KMSS] tells us that for almost every realization of the random field $(V(x), x \in \mathbb{Z}^d)$ (now $V(x) = \pm 1$) and for all $x \in \mathbb{Z}^d$

$$\lim_{k \uparrow \infty} \frac{1}{k} \ln \mathbf{E}_{x_0 = x}\left[\exp\left(\lambda \sum_{n=0}^{k-1} V(x(n))\right)\right] = \lambda \tag{6.7}$$

while the formal perturbation series would start with a term of order λ^2. This means that the spectrum of H^λ is shifted by $\mathrm{O}(\lambda)$ with respect to that of the Laplacian and that an argument based on perturbation theory for the existence of the weak-coupling limit $t \simeq \lambda^{-2}$ should not be trusted.

A more physical way of expressing all this may be to argue that the behaviour is not purely the scattering we might expect; there is a finite amplitude for the particle getting trapped in a bound state. A block of N^d sites all having potential $V(x) = -V$ will give a bound state if N is sufficiently large. The presence of loops makes this bound state available.

7. Conclusions

We have considered the problem of the van Hove weak-coupling limit for a quantum particle undergoing impurity scattering. For a directed lattice (tree) we have calculated the limit explicitely. For the regular lattice we have argued that this limit does not exist.

Our methods are based on a rigorous relation that we established between the quantum problem and the problem of a random walk in a random environment. This approach is non-perturbative and distinguishes itself from the usual Dyson-series approach which has worked in the continuum case, which has not worked in the lattice case (see the mistakes and gaps in the 'proofs' in [ME] and [Hug]), and which, as we argued, may fail in the lattice case.

Acknowledgments

We have very much profited from discussions with N Angelescu, B Tóth, M Fannes, O Penrose and H Spohn. We further thank the referees whose comments were very helpful. WS wants to thank the Instituut voor Theoretische Fysica (KU Leuven), especially A Verbeure, for their very kind hospitality and financial support. WS also acknowledges financial support from the EC under the ERASMUS Project. This work is partially supported by the EC under grant No CHRX-CT93-0411.

Appendix. Analysis of section 6.2

Here we work out the weak-coupling limit for the example of the linear chain of section 6.2. We recall that the expectation

$$\mathbf{E}_V\left[\left(\frac{1}{p+\mathrm{i}\lambda V}\right)^l\right] = \frac{1}{2}\left(\frac{1}{p+\mathrm{i}\lambda}\right)^l + \frac{1}{2}\left(\frac{1}{p-\mathrm{i}\lambda}\right)^l.$$

We will work with the constant function $f \equiv a$; $\mathrm{e}^{-\mathrm{i}t\Delta} f$ is then equal to a.

At first we have to deal with the sums

$$\begin{aligned}
&\frac{1}{2}a\sum_{k=1}^{\infty}\mathrm{i}^k\sum_{l=0}^{k-1}\left(\frac{1}{2}\right)^{l+1}\left(\frac{1}{p\pm\mathrm{i}\lambda V}\right)^{l+1}\left(\frac{p}{p^2+\lambda^2V^2}\right)^{k-l} + \frac{1}{2}a\sum_{k=0}^{\infty}\left(\frac{\mathrm{i}}{2}\right)^k\left(\frac{1}{p\pm\mathrm{i}\lambda V}\right)^{k+1}\\
&\qquad = \frac{1}{4}a\frac{1}{p\pm\mathrm{i}\lambda V}\sum_{k=1}^{\infty}\left(\frac{\mathrm{i}p}{p^2+\lambda^2V^2}\right)^k\sum_{l=0}^{k-1}\left(\frac{1}{2}\frac{p\mp\mathrm{i}\lambda V}{p}\right)^l\\
&\qquad\quad +\frac{1}{2}a\frac{1}{p\pm\mathrm{i}\lambda V}\sum_{k=0}^{\infty}\left(\frac{\mathrm{i}}{2(p\pm\mathrm{i}\lambda V}\right)^k\\
&\qquad = \frac{1}{4}a\frac{1}{p\pm\mathrm{i}\lambda V}\sum_{k=1}^{\infty}\left(\frac{ip}{p^2+\lambda^2V^2}\right)^k\cdot\frac{1-(\frac{1}{2}(p\mp\mathrm{i}\lambda V)/p)^k}{1-\frac{1}{2}(p\mp\mathrm{i}\lambda V)/p}\\
&\qquad\quad +\frac{1}{2}a\frac{1}{p\pm\mathrm{i}\lambda V}\frac{1}{1-\mathrm{i}/\big(2(p\pm\mathrm{i}\lambda V)\big)}\\
&\qquad = \frac{1}{4}a\frac{1}{p\pm\mathrm{i}\lambda V}\left[\frac{\mathrm{i}p/p^2+\lambda^2V^2}{1-\mathrm{i}p/p^2+\lambda^2V^2} - \frac{\frac{1}{2}\mathrm{i}(p\pm\mathrm{i}\lambda V)}{1-\frac{1}{2}\mathrm{i}(p\pm\mathrm{i}\lambda V)}\right]\\
&\qquad\quad \times\frac{1}{1-\frac{1}{2}(p\mp\mathrm{i}\lambda V)/p} + \frac{1}{2}a\frac{1}{p\pm\mathrm{i}\lambda V-\frac{1}{2}\mathrm{i}}\\
&\qquad = \frac{1}{2}a\left[\frac{\mathrm{i}p}{p^2-\mathrm{i}p+\lambda^2V^2} - \mathrm{i}\frac{p\pm\mathrm{i}\lambda V}{p\pm\mathrm{i}\lambda V-2\mathrm{i}}\right]\frac{p}{(p\pm\mathrm{i}\lambda V)^2} + \frac{1}{2}a\frac{1}{p\pm\mathrm{i}\lambda V-\frac{1}{2}\mathrm{i}}.
\end{aligned}$$

This is exactly equation (6.4) of section 6.2.

References

[C] Carmona R 1984 *Random Schrödinger operators (Lecture Notes in Mathematics 1180)* p 53

[FV] Feynman R P and Vernon F L 1963 The theory of a general quantum system interacting with a linear dissipative system *Ann. Phys.* **24** 119

[HLW] Ho T G, Landau L J and Wilkins A J 1993 On the weak-coupling limit for a Fermi gas in a random potential *Rev. Math. Phys.* **5** 209

[Hov] van Hove L 1955 Quantum-mechanical perturbations giving rise to a statistical transport equation *Physica* **21** 517

[Hug] Hugenholtz N M 1983 Derivation of the transport equation for a Fermi gas *J. Stat. Phys.* **32** 231

[KMSS] Khanin K M, Mazel A E, Shlosman S B and Sinai Ya G Loop condensation effects in the behaviour of the random walks *Preprint*

[KV] Kipnis C and Varadhan S R S 1986 A central limit theorem for additive functionals of reversible Markov processes and applications to simple exclusion *Commun. Math. Phys.* **106** 1

[Lan] Landau L J 1994 Weak coupling limit: Feynman diagrams 53 *On Three Levels* ed M Fannes, C Maes and A Verbeure

[ME] Martin Ph and Emch G G 1975 A rigorous model sustaining van Hove's phenomenon *Helv. Phys. Acta* **48** 59

[MFGW] DeMasi A, Ferrari P A, Goldstein S and Wick W D 1989 An invariance principle for reversible Markov processes. Applications to random motions in random environments *J. Stat. Phys.* **55** 787

[Spo] Spohn H 1977 Derivation of the transport equation for electrons moving through random impurities *J. Stat. Phys.* **17** 385