Kinetic Equations for Quantum Many-Particle Systems

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1 The framework

Kinetic equations are a widely used and highly successful method to understand dynamical aspects of quantum many particle systems. As a standard reference I mention the book by Ziman [1] which in large parts is based on the kinetic method.

My article deals with the issue to derive such an equation in a well-defined limit from quantum dynamics. For sake of a simple presentation I restrict myself to a weak interaction potential. There is a parallel discussion for low density for which I have to point to the literature [2, 3]. Let me first describe the general framework in admittedly rather vague terms. The broad picture will be made precise in the remainder of the article, where also the border between proven and conjectured will be traced out.

We consider (nonrelativistic) quantum particles moving in three dimensions and interacting through a short range potential. The Hamiltonian is of the generic form

\[ H = H_0 + \sqrt{\varepsilon} H_1, \]  

(1.1)

where \( H_0 \) denotes the free Hamiltonian. \( H_1 \) is the interaction which is multiplied by a dimensionless strength parameter \( \sqrt{\varepsilon} \). We want to study a system of many particles and, first, consider a spatially homogeneous situation, which is idealized as an infinitely extended system in a spatially translation invariant state. Amongst the many conceivable states there is a special class of states characterized by being quasifree, translation invariant, and time-invariant under the dynamics generated by \( H_0 \). Such a state is uniquely characterized by a mass density \( \rho > 0 \), and a momentum distribution \( W(k)/\rho, \int dkW(k) = \rho \).

Under the full dynamics generated by \( \dot{H} \) such a quasifree state changes in time but remains translation invariant. The change is slow, since the interaction is weak. By definition, the kinetic time scale is the shortest scale over which the change in the momentum distribution is of order 1. Since transition rates are roughly proportional to \( |\sqrt{\varepsilon} H_1|^2 \), the kinetic time scale should be \( \varepsilon^{-1} t \), in microscopic time units. On the kinetic time scale the momentum distribution evolves according to an autonomous nonlinear transport equation. Generically, on the basis of this equation, the long time limit will be the thermal equilibrium momentum distribution for \( H_0 \), i.e. for the noninteracting particles. Moreover, the kinetic equation makes a quantitative prediction on how thermal equilibrium is approached.

At this stage the difficulty of a proof becomes already apparent. Since \( \varepsilon \ll 1 \), Equation (1.1) looks like a standard perturbation problem. But this perturbation has to be controlled over the very long times \( \varepsilon^{-1} t \).

What happens if the initial state is not quasifree but still translation invariant? This situation is analysed in [4] for a weakly interacting Fermi gas on a lattice. If the initial state has good spatial clustering, then, under the \( H_0 \)-dynamics for long microscopic times, the state becomes quasifree without yet changing the momentum distribution. The resulting dynamical picture is rather compelling: For “reasonable” initial states, the time-evolved state becomes rapidly quasifree. At kinetic times the
interaction makes itself felt, changing the momentum distribution but maintaining the quasifree property. At even longer times the system presumably tries to establish the equilibrium state for $H$, which is not strictly quasifree. For fixed small $\varepsilon$, physically the time scales are not perfectly separated. But mathematically, a separation can be achieved through taking limits. The first regime is $\varepsilon = 0$ and $t \to \infty$. The kinetic regime is $\varepsilon \to 0$ and $t \to \infty$, $\varepsilon t = \tau$ fixed, while the third regime is $\varepsilon$ fixed and small, while $t \to \infty$. Needless to remark that the third regime is inaccessible mathematically.

Usually, one also wants to include spatial variations, which however are slow on the scale of the typical distance between particles. For such slow variations, the $H_0$-dynamics can be approximated by semiclassics, which means that particles move independently with classical kinetic energy $\omega(k)$, $\omega$ being the dispersion relation for the quantum particles. The kinetic time scale has been determined already. To have the $H_0$-dynamics of the same order as the collisions requires then a spatial variation of order $\varepsilon^{-1}$ in microscopic units. The momentum distribution varies now spatially on the kinetic scale. Thus $W(k)$ is to be replaced by $W(r,k)$. The collision term is strictly local in $r$, while the kinetic equation picks up the flow term $-\nabla_k \omega(k) \cdot \nabla_r W(r,k)$ from the semiclassical approximation. Close to $r$ the microscopic state is still quasifree and translation invariant, at least in approximation.

2 Model hamiltonians

There is some freedom in the choice of the microscopic model. Firstly, the position space is either $\mathbb{R}^3$ or some Bravais lattice which we take to be $\mathbb{Z}^3$. (We will comment on the spatial dimension below.) The average number of particles is finite but diverges as $\varepsilon^{-3}$ in the kinetic limit. Thus the Hilbert space for the system is the boson Fock space $\mathcal{F}_+$, resp. fermion Fock space $\mathcal{F}_-$, over either $L^2(\mathbb{R}^3)$ or $l^2(\mathbb{Z}^3)$. Let $a(x)$, $a(x)^*$, $x \in \mathbb{R}^3$, resp. $x \in \mathbb{Z}^3$, denote annihilation and creation operators for the Bose, resp. Fermi, fields. Setting $\hbar = 1$, they satisfy the commutation relations

$$[a(x), a(x')]_\mp = 0 = [a(x)^*, a(x')^*]_\mp,$$

$$[a(x), a(x')^*]_\mp = \delta(x - x'),$$

where $[\cdot, \cdot]_-$ denotes the commutator, $[\cdot, \cdot]_+$ the anticommutator, and $\delta(x - x')$ stands for the Kronecker $\delta$ in case of $\mathbb{Z}^3$. The momentum space operators are distinguished only through their argument and given by

$$a(k) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} dx e^{-ik \cdot x} a(x), \quad k \in \mathbb{R}^3,$$

$$a(k) = \sum_{x \in \mathbb{Z}^3} e^{-i2\pi k \cdot x} a(x), \quad k \in [-\frac{1}{2}, \frac{1}{2}]^3 = \mathbb{T}^3.$$  

(i) Independent particles with random impurities (Anderson model). Particles hop
to nearest neighbor sites and are subject to a static potential $V(x)$. Then the hamiltonian reads

$$H = -\frac{1}{2} \sum_{x \in \mathbb{Z}^3} a(x)^*(\Delta a)(x) + \sqrt{\varepsilon} \sum_{x \in \mathbb{Z}^3} V(x)a(x)^*a(x). \quad (2.5)$$

Here $\Delta$ is the lattice Laplacian and $\{V(x), x \in \mathbb{Z}^3\}$ is a collection of independent random variables. The random potential mimics the interaction. The kinetic equation will be linear, however.

(ii) Electron-phonon systems. $a(x)$ is the Fermi field of the electrons and $c(x)$ is the Bose field of the phonons. The hamiltonian is given by

$$H = -\frac{1}{2} \int_{\mathbb{R}^3} dx a(x)^* \Delta a(x) + \int_{\mathbb{R}^3} dk \omega(k) c(k)^*c(k)$$

$$+ \sqrt{\varepsilon} \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dx' a^*(x)a(x)g(x-x')(c(x') + c(x')^*) \quad (2.6)$$

with $\omega$ the phonon dispersion and $g$ a suitable coupling function. The number of electrons is conserved. Assuming the phonon system to be infinitely extended and in thermal equilibrium, the dynamics of a single electron is governed by a linear kinetic equation.

(iii) Weakly interacting fermions and bosons. If the pair potential is denoted by $V$, the hamiltonian reads

$$H = -\frac{1}{2} \int_{\mathbb{R}^3} dx a(x)^* \Delta a(x) + \int_{\mathbb{R}^6} dx dx' a^*(x)a(x') V(x-x')a(x)a(x'). \quad (2.7)$$

(iv) Phonons. Phonons are bosons. For effective single band models the free part is of the form

$$H = \int_{\mathbb{T}^3} dk \omega(k)a(k)^*a(k). \quad (2.8)$$

$\omega$ is the dispersion relation. $\omega^2$ is the Fourier transform of a rapidly decaying lattice function. For an acoustic band $\omega(k) = |k|$ for small $k$, while for optical bands $\omega(k) \geq \omega_0 > 0$ for all $k \in \mathbb{T}^3$. Expanding around the harmonic potentials yields cubic and quartic nonlinearities. For example, a quartic on-site potential would be $\lambda \sum_{x \in \mathbb{Z}^3}(q_x)^4$, $q_x$ the scalar displacement at $x$ away from the equilibrium position, while cubic nonlinear springs correspond to $\frac{1}{3} \sum_{x,y \in \mathbb{Z}^3} \alpha(x-y)(q_x - q_y)^3$. The respective interaction hamiltonians are

$$H_{14} = \lambda \int_{\mathbb{T}^{12}} dk_1dk_2dk_3dk_4 \delta(k_1+k_2+k_3+k_4) \prod_{j=1}^4 (2\omega(k_j))^{-1/2} (a(k_j)+a(-k_j)^*) \quad (2.9)$$
\[ H_{13} = \frac{1}{3} \int_{T^3} dk_1 dk_2 dk_3 \delta(k_1 + k_2 + k_3) \sum_{x \in \mathbb{Z}^3} \alpha(x) \prod_{j=1}^{4} \left( 2\omega(k_j)^{-1/2} (e^{i 2\pi k_j \cdot x} - 1) (a(k_j) + a(-k_j)^*) \right). \] (2.10)

\[ H_0 + \sqrt{\varepsilon} H_{13} \] is not bounded from below, a defect not yet seen on the kinetic time scale. For phonon systems the particle number is not conserved. However, it is possible that on the kinetic level only processes with number conservation are allowed.

### 3 Initial state

As explained in Section 1, for the spatially homogeneous case the initial state is translation invariant, quasifree, and invariant under the \( H_0 \) dynamics. Therefore \( \langle a(k) \rangle = 0 = \langle a(k)^* \rangle \) and

\[ \langle a(k')^* a(k) \rangle = W(k) \delta(k - k'), \quad \langle a(k')^* a(k)^* \rangle = 0, \quad \langle a(k'^*) a(k) \rangle = 0. \] (3.1)

Here \( W(k) \geq 0 \) and for fermions in addition \( W(k) \leq 1 \). All other moments are determined through the two-point function, i.e.

\[ \langle \prod_{j=1}^{m} a(k_j^*) \prod_{j=1}^{m} a(k_j') \rangle = \frac{\text{per}}{\det} \{ \langle a(k_i^*) a(k_j) \rangle \}^{i,j=1,...,m} \] (3.3)

with all other monomials having vanishing expectation. Such a state has infinite energy and is not supported on Fock space.

To model the spatially inhomogeneous situation, we give ourselves a spatially dependent Wigner function \( W(r, k) \), \( W(r, k) \geq 0, W(r, k) \leq 1 \) for fermions, and of rapid decay, in particular \( \int dr \int dk W(r, k) < \infty \). Secondly we choose a sequence of trace class operators, \( R^\varepsilon, \varepsilon > 0 \), on \( \mathcal{F}, R^\varepsilon \geq 0 \) and \( R^\varepsilon \leq 1 \) for fermions. Let \( R^\varepsilon(x, y) \) be the corresponding integral kernel. Then the sequence of initial states, \( \langle \cdot \rangle_\varepsilon, \varepsilon > 0 \), still satisfies (3.1), (3.2), and (3.3) with

\[ \langle a(x)^* a(y) \rangle_\varepsilon = R^\varepsilon(x, y). \] (3.4)

The Wigner function \( W \) appears through the limit \( \varepsilon \to 0 \) by requiring

\[ \lim_{\varepsilon \to 0} R^\varepsilon \left( \varepsilon^{-1} r + \frac{1}{2} \eta, \varepsilon^{-1} r - \frac{1}{2} \eta \right) = \int_{\mathbb{R}^3} dk e^{ik \cdot \eta} W(r, k). \] (3.5)

In particular, for the number of particles, \( N \), one has

\[ \langle N \rangle_\varepsilon \approx \varepsilon^{-3}. \] (3.6)
\( \text{(3.5)} \) implies that at \( r \), on the kinetic scale, in the limit \( \varepsilon \to 0 \) the state is quasifree with correlator \( W(r, k)\delta(k - k') \) (\( r \) is fixed here). Spatial averages on the kinetic scale are self-averaging (law of large numbers). To see this, let \( A \) be a local observable and \( \tau_x \) the shift by \( x \). Spatial average on the kinetic scale means

\[
\varepsilon^3 \int_{\mathbb{R}^3} dx \chi_\Lambda(\varepsilon x) \tau_x A = n^\varepsilon(\Lambda, A) \tag{3.7}
\]

with \( \chi_\Lambda \) the indicator function of a fixed box \( \Lambda \). Then

\[
\lim_{\varepsilon \to 0} n^\varepsilon(\Lambda, A) = \int_{\mathbb{R}^3} dr \chi_\Lambda(r) \langle A \rangle_{W(r, \cdot)} \tag{3.8}
\]

in the sense that the variance of \( n^\varepsilon(\Lambda, A) \) vanishes as \( \varepsilon \to 0 \). \( \langle A \rangle_{W(r, \cdot)} \) is here the average of \( A \) in the translation invariant, quasifree state with correlator

\[
\langle a(k')^* a(k) \rangle_{W(r, \cdot)} = W(r, k)\delta(k - k') \tag{3.9}
\]

### 4 Kinetic limit

Let \( U^\varepsilon(t) = \exp[i(H_0 + \varepsilon H_1)t] \) be the unitary group generated by \( H \). (In brackets we note that in all models \( H \) is self-adjoint with domain \( D(H_0) \) under reasonable assumptions on the coefficients, except for \( H_0 + \sqrt{\varepsilon}H_{13} \) which has to be stabilized by adding a small quartic potential.) As initial state we choose the sequence \( \langle \cdot \rangle_\varepsilon \) of quasifree states from Section 3. It is time evolved to \( \langle \cdot \rangle_\varepsilon(t) \) according to \( \langle A \rangle_{W(r, \cdot)} = \langle U^\varepsilon(t)^* AU^\varepsilon(t) \rangle_\varepsilon \) for all \( A \in B(\mathcal{F}) \). To prove the kinetic limit firstly means to establish the existence of

\[
\lim_{\varepsilon \to 0} \langle a(\varepsilon^{-1}r - \frac{1}{2}\eta)^* a(\varepsilon^{-1}r + \frac{1}{2}\eta) \rangle_{\varepsilon}(\varepsilon^{-1}t) = \int_{\mathbb{R}^3} dk e^{ik\cdot\eta} W(r, k, t) . \tag{4.1}
\]

(For model (i) one averages also over the random potential. For model (ii) one considers only a single electron and averages over the thermal state of the phonons.) Clearly an issue is the sense in which the limit (4.1) is intended. Usually one proves weak convergence, but pointwise convergence could hold. More ambitiously one can study higher moments which should follow the pattern explained in Section 3. Only the Wigner function \( W(r, k) \) is to be replaced by the time-evolved Wigner function \( W(r, k, t) \). A further item would be the law of large numbers and its central limit corrections.

Secondly the time evolution of the Wigner function \( W(r, k, t) \) must be governed by an autonomous transport equation. If \( H_1 = 0 \), such a property and the limit (4.1) are easily established with the result

\[
\frac{\partial}{\partial t} W(r, k, t) + \nabla_k \omega(k) \cdot \nabla_r W(r, k, t) = 0 . \tag{4.2}
\]
If $H_1 \neq 0$, the transport equation (4.2) acquires a collision term as

$$\frac{\partial}{\partial t} W(r, k, t) + \nabla_k \omega(k) \cdot \nabla_r W(r, k, t) = C(W)(r, k, t). \quad (4.3)$$

The collision operator $C$ is local in space-time and we only have to display its action on the momentum variable. Of course $C$ depends on the particular model. Let us give only two examples. For an electron in a random potential one obtains

$$C(W)(k) = 2\pi \int_{\mathbb{R}^3} dk' \hat{\vartheta}(k - k') \delta(\omega(k) - \omega(k')) (W(k') - W(k)). \quad (4.4)$$

Here $\omega$ is the dispersion relation for the electron and $\hat{\vartheta}$ is the Fourier transform of the correlator of the random potential, $\vartheta(x - x') = \langle V(x)V(x') \rangle$, $\langle V(x) \rangle = 0$. The collisions uniformize the momentum over the shell of constant energy. Thus with this collision term Eq. (4.3) has the property that as $t \to \infty$ the distribution function of the electron converges to $W(k) = \delta(\omega(k) - E)$, given the initial data have kinetic energy $E$.

Our second example is the Uehling-Uhlenbeck equation for weakly interacting quantum fluids [5], example (iii), which for fermions was first derived by Nordheim [6]. The collision term reads

$$C(W)(k_1) = \int dk_2 dk_3 dk_4 \Phi(k_1, k_2|k_3, k_4)
\left[ W_3 W_4 (1 + \theta W_1)(1 + \theta W_2) - W_1 W_2 (1 + \theta W_3)(1 + \theta W_4) \right], \quad (4.5)$$

$W_j = W(k_j)$, with $\theta = 1$ for bosons and $\theta = -1$ for fermions. The collision rate encodes energy-momentum conservation and the interaction potential in the Born approximation as

$$\Phi(k_1, k_2|k_3, k_4) = |\tilde{V}(k_1 - k_3) + \theta \tilde{V}(k_2 - k_3)|^2 \delta(k_1 + k_2 - k_3 - k_4)
\delta(\omega_1 + \omega_2 - \omega_3 - \omega_4), \quad \omega_j = \frac{1}{2}k_j^2. \quad (4.6)$$

Note that (4.5) is in fact cubic. The added term makes symmetry of the collision operator more transparent. Phonon collision operators are listed in [7]. They were first derived by Peierls [8].

One part of the limit theorem must ensure the existence of a unique solution to the transport equation (4.3). For a linear collision operator tools are available. For a nonlinear collision operator local in time existence can always be established. To have a solution global in time is a difficult issue. Since collisions are at some particular spatial location, the nonlinearity is well-defined only if $\sup_{r,k} W(r,k,t)$ is bounded, a property one does not know how to establish in generality. An exception are fermions governed by (4.5) with $\theta = -1$. Then the solution must satisfy $0 \leq W(r,k,t) \leq 1$ for all $t$, see [9] for a complete discussion.
5 Mathematical results

For a classical system of hard spheres at low density all facets of the kinetic limit are proved under the sole restriction of kinetically short times, i.e. $|t| \leq t_0 = 1/5$-th of the mean free time [10], see also [11, 12]. The issue under discussion is to carry out a corresponding program for weakly nonlinear wave equations, resp. linear wave equations with weak disorder.

The zeroth order step is to have a convincing formal derivation and thereby to determine the collision operator. Such formal derivations abound in the physics literature. They span from a direct application of Fermi’s golden rule to sophisticated diagrammatic expansions. To me the most convincing argument is a truncation procedure based on the assumption that the state at microscopic time $\varepsilon^{-1}t$ is approximately quasifree. The details can be found in [13], see also [14], for weakly interacting quantum fluids and in [7] for weakly interacting phonons.

Up to now, any proof is based on the time-dependent perturbation theory, which means to expand

$$e^{-iHt} = e^{-iH_0t} + \sum_{n=1}^{\infty} \int_{0\leq t_1\leq \ldots \leq t_n \leq t} dt_1 \ldots dt_n e^{-iH_0(t-t_n)} V_1 \ldots V_i e^{-iH_0t_1}. \quad (5.1)$$

Inserting in $\langle U(t)^* a(y)^* a(x) U(t) \rangle_\varepsilon$ and working out the average over the initial state (resp. over the random potential) this expectation is then represented as a sum of high-dimensional oscillatory integrals (= diagrams). Very crudely the next two steps consist in dividing between

- leading diagrams. Their $\varepsilon \to 0$ limit does not vanish.
- subleading diagrams. Their $\varepsilon \to 0$ limit vanishes.

Since (5.1) is an infinite series, one needs on top

- a uniform bound on the series.
- the leading diagrams at $\varepsilon = 0$ sum to the time-dependent solution of the transport equation.

There are variations in the way how to arrange the perturbation series. The expansion of $\langle U(t)^* a(y)^* a(x) U(t) \rangle_\varepsilon$ yields standard Feynman diagrams. Particle conservation is exploited more efficiently by considering the hierarchy of $n$-particle Wigner functions, $n = 1, 2, \ldots$ [14, 15, 16]. For a particle in a random potential the most powerful method is to use directly (5.1) [17].

A second basic choice is between $\mathbb{R}^3$ and $\mathbb{Z}^3$ as position space. $\mathbb{R}^3$ has the advantage that for phase factors of the form $e^{-ik^2t}$ the oscillatory integrals are easily estimated. On the other hand the large $k$ behavior needs extra efforts. For $\mathbb{Z}^3$ the free propagator is less explicit, but momentum space is $\mathbb{T}^3$, hence bounded.
For weakly interacting systems the perturbation series diverges on the kinetic time scale. This leaves one with analysing individual diagrams. For a translation invariant Fermi gas all terms up to order $(V_1)^2$ are studied [4] and the approximation $W(k, t) = W(k) + t\mathcal{C}(W)(k)$ is proved with $\mathcal{C}$ of (1.5) for $\theta = -1$ and integrations over $\mathbb{T}^3$, $\omega(k) = \sum_{j=1}^3 (1 - \cos k^j)$. For bosons and fermions moving in $\mathbb{R}^3$ the same result is obtained for spatially inhomogeneous initial data [15]. The next set of results concerns the analysis of a certain subclass of diagrams, e.g., all leading diagrams [14] or the identity permutation in (3.3) which corresponds to Boltzmann statistics [18]. All these results strongly support the kinetic picture. Spatial dimension has to be larger than three, which roughly comes from conditions on oscillatory integrals as, e.g.,

$$ \int_0^\infty dt | \int_{\mathbb{T}_d} dke^{-i\omega(k)t} | < \infty. $$

(5.2)

For the motion in a random potential the situation is more favorable. Assume a Gaussian random potential. Then only even moments contribute. For the $2n$-th term of the perturbation series this yields a bound as $\frac{1}{n!}\varepsilon^n (\varepsilon^{-1} t)^n c^n ((2n)!/2^n n!)$, where the term in the second round brackets comes from the number of pairings for the Gaussian random potential. Thus the perturbation series has a finite radius of convergence, $t_0$, on the kinetic scale. With this restriction the kinetic program can be carried through. The spatially homogeneous case is dealt with in [19], which is substantially improved and extended in [20], see also the discussion in [21]. In 1997 L. Erdős and H.-T. Yau [22] announced a truly remarkable breakthrough. By a suitable truncation of the perturbation series, the remainder being controlled by unitarity, they succeed to prove the kinetic limit for arbitrary $t_0$. With their technique other cases can be handled as well, to list: low density scatterers [23], non-Gaussian but approximately independent random potentials [24], tight binding dynamics [25], coupling to a phonon bath [26], and mass disordered lattice dynamics [27]. Chen proves self-averaging [28] and the link to spectral properties of $H$ [25].

Staying in the context of the motion of an electron in a random potential, one might wonder what happens beyond the kinetic time scale. Mathematically this means to consider times of order $\varepsilon^{-(1+\alpha)} t$ in microscopic units with $\alpha > 0$ in the limit $\varepsilon \to 0$. This implies very long kinetic times at which the solution to the transport equation is already of the form

$$ W(r, k, t) \cong \rho(r, t) \delta(E - \omega(k)) $$

(5.3)

with $E$ determined by the initial conditions. The mass density $\rho$ has a slow variation and is governed by the diffusion equation

$$ \frac{\partial}{\partial t} \rho(r, t) = D_{\text{kin}}(E) \Delta_r \rho(r, t), $$

(5.4)

where $D_{\text{kin}}(E)$ is the energy dependent diffusion coefficient of the kinetic equation

$$ \frac{\partial}{\partial t} W(r, k, t) + \nabla_k \omega(k) \cdot \nabla_r W(r, k, t) = \mathcal{C}(W)(r, k, t) $$

(5.5)
with $\mathcal{C}$ the collision operator from (1.4). If $\alpha$ is large, the diffusion coefficient in (5.4) should be close to the diffusion coefficient as computed for fixed small $\varepsilon$, which is definitely different from $D_{\text{kin}}(E)$. Thus there must be a critical $\alpha_c$ up to which (5.3) together with (5.4) is valid. The theoretical prediction is $\alpha_c = 1$. Erdős, Salmhofer, and Yau \cite{29,30} prove (5.3), (5.4) for $0 < \alpha < 10^{-3}$.

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