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SEMICLASSICAL APPROXIMATION OF ELECTRON-PHONON SCATTERING BEYOND FERMI'S GOLDEN RULE*

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Abstract. We derive a quantum mechanical correction to the semiclassical Fermi golden rule operator for scattering of electrons in a crystal. This correction takes into account the fact that electron-phonon interaction is not instantaneous in quantum mechanics. The corrective term is derived via an oscillatory, i.e., weak, limit in the Levinson equation for large timescales.

Key words. asymptotic analysis, quantum mechanics, Levinson equation, Wigner functions, Fermi's golden rule, Boltzmann equation

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1. Introduction.

It is generally accepted that the dominant collision mechanism for electron transport in crystals is scattering of electrons by phonons, i.e., with vibrations of the crystal lattice. In a semiclassical description this collision mechanism is described by the Fermi golden rule. In the absence of an electric field and in the spatially homogeneous case, the evolution of the effective single electron density function is then given by the Boltzmann equation

$$\begin{aligned} &\text{(a)} \quad \partial_t f(p,t) = Q_{FGR}[f](p,t) \\ &\qquad\qquad := \int dp' [S_{FGR}(p,p') f(p',t) - S_{FGR}(p',p) f(p,t)], \\ &\text{(b)} \quad S_{FGR}(p,p') = [A^- \delta(\varepsilon(p) - \varepsilon(p') - \hbar\omega) + A^+ \delta(\varepsilon(p) - \varepsilon(p') + \hbar\omega)], \end{aligned} \tag{1.1}$$

where p denotes the momentum vector and $\varepsilon(p) = \frac{|p|^2}{2m_*}$ denotes the energy associated with the momentum p. The Fermi golden rule states that during a collision the electron gains or loses an amount $\hbar\omega$ of energy from the crystal lattice by annihilation or generation of a phonon. We remark that the Boltzmann equation (1.1) models instantaneous collisions; i.e., the momentum of an electron changes instantaneously from p' to p during a collision event.

Semiclassical transport theory based on the Boltzmann equation neglects several effects which originate from the quantum mechanical nature of the charge carriers, such as a collisional broadening due to the finite lifetime of the carrier momentum eigenstate, collision retardation, and the intracollisional field effect due to the action of the electric field during the scattering process [11]. To describe these effects a quantum kinetic equation has to be adopted which takes the finiteness of the scattering duration into account. An appropriate kinetic equation describing the interaction of a single electron with the equilibrium phonon system of a semiconductor has been proposed

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by Levinson [6]. Restricting ourselves to the case of a spatially uniform semiconductor and vanishing electric field, the Levinson equation is of the form

$$
\begin{aligned}
&\text{(a)} \quad \partial_t f(p,t) = Q[f](p,t) \\
&\qquad\qquad := \int_0^t dt' \int dp' [S(p,p',t-t')f(p',t') - S(p',p,t-t')f(p,t')], \\
&\text{(b)} \quad S(p,p',t) = \frac{2VF^2 n}{(2\pi\hbar)^3} \cos\left[\frac{t}{\hbar}(\varepsilon(p) - \varepsilon(p') - \hbar\omega)\right] \\
&\qquad\qquad + \frac{2VF^2(n+1)}{(2\pi\hbar)^3} \cos\left[\frac{t}{\hbar}(\varepsilon(p) - \varepsilon(p') + \hbar\omega)\right], \\
&\qquad \varepsilon(p) = \frac{|p|^2}{2m_*}, \quad n = \frac{1}{\exp(\beta\hbar\omega) - 1}.
\end{aligned} \tag{1.2}
$$

The symbols in (1.2) have the following meaning: $\hbar F$ denotes the electron-phonon interaction matrix element, $\hbar\omega$ the phonon energy, V the normalization volume, m_* the effective electron mass, n the Bose–Einstein distribution, and $\beta = (k_B T)^{-1}$ the inverse temperature of the phonon system. Note that, other than the Fermi golden rule equation (1.1), the Levinson equation (1.2) is nonlocal in time, and the effect of a collision is actually felt for all future times. Therefore the Levinson equation is able to model some of the effects mentioned above, which become increasingly relevant as the dimensions of modern semiconductor devices decrease, and, consequently, fast relaxation processes play a more prominent role. The Levinson equation can be derived from the quantum mechanical many body problem for one electron and an arbitrary number of phonons, i.e., from an infinite system of Schrödinger equations for the wave functions $\psi_n(p, q_1, \ldots, q_n, t)$, where p is the electron momentum vector and the q_j denote the phonon momenta. ψ_n describes the state of the system for one electron and n phonons, and ψ_n is coupled to ψ_{n-1} and ψ_{n+1} via coupling terms in the Fröhlich Hamiltonian, modelling the creation and annihilation of phonons. The function f is then the Wigner function corresponding to the phonon trace of the density matrix. We refer the reader to [1], [3], [4], [5] for an overview of the derivation. The Levinson equation represents the weak coupling limit of this system, which means that only electron-phonon interactions of first order are retained. An interaction starts at some time, say t_1, when one half of the phonon momentum is transferred to the electron, and gets completed at some time t_2, when the second half of the phonon momentum is transferred (see, e.g., [4], [9]). These partial processes capture the emission and absorption of both real and virtual phonons. The weak coupling limit implies that during the period $t_2 - t_1$ of a particular interaction no other interaction can start. In other words, only a sequence of completed interactions is considered. The time between two interactions is determined by the frequency F given by the interaction matrix element, whereas the duration of the interaction depends on the frequency of the lattice vibrations, ω. Therefore, $F \ll \omega$ must hold. A result of the weak coupling limit is that no powers higher than F^2 appear in (1.2)(b). To our knowledge, a completely rigorous mathematical derivation of the Levinson equation from the many body problem for the Fröhlich Hamiltonian is still outstanding. However, for the purpose of this paper, we will assume the Levinson equation (1.2) to be valid.

Remark: The Levinson equation results from an asymptotic expansion of the Fröhlich Hamiltonian for small coupling coefficients [1], [3]. While there obviously is a density matrix formulation of the Levinson equation, which is given by the Fourier

transform of (1.2), the corresponding density matrix cannot simply be written as a superposition of pure state wave functions, and therefore the positive definiteness of the Wigner function f in (1.2) cannot be guaranteed automatically.

The objective of the present paper is to relate (1.2) to the Fermi golden rule (1.1). While much simpler than the original many body equation, the Levinson equation still poses significant challenges because of its nonlocality in time and rapid oscillations due to the presence of the term $t/\hbar$ in the integral kernel in (1.2). It is mentioned in the original work [6] that in the classical limit $\hbar \to 0$ the scattering rate S in (1.2)(b) will be replaced by the Fermi golden rule (cf. [2]).

In the present paper we prove the convergence of the Levinson operator Q in (1.2) to the Fermi golden rule operator Q_{FGR} for large timescales, and more importantly, in addition to the golden rule the first order term in the asymptotic expansion is derived. The result is a correction to the Fermi golden rule, which better reflects the effects of finite collision times. The resulting corrected operator is structurally of the form

$$Q_C[f] = \int dp' [S_C(p, p', \partial_t) f(p', t) - S_C(p', p, \partial_t) f(p, t)], \tag{1.3}$$

where the corrected scattering rate S_C contains the Fermi golden rule rate S_{FGR} and a correction term that involves the time derivative of the density function. However, the corrected operator Q_C in (1.3) is still local in time, in the sense that it is not an integral operator in time, and therefore the resulting transport equation is much simpler to solve than the Levinson equation (1.2). More precisely, we prove that the Levinson operator Q converges weakly, in zeroth order to Q_{FGR}, and in first order to the corrected operator Q_C. The considered regime is one of large timescales, i.e., timescales which are much larger than $1/\omega$, where ω is the frequency with which the lattice vibrates.

This paper is organized as follows. In section 2 we introduce an appropriate dimensionless form of the Levinson equation (1.2) which contains a dimensionless parameter $\lambda = (\omega t_0)^{-1}$, where t_0 is the timescale under consideration. Section 3 contains the asymptotic analysis for $\lambda \to 0$. We prove that $Q = Q_C + o(\lambda)$, $Q_C = Q_{FGR} + \lambda Q_1$ holds in a weak sense, i.e., when integrated against a fixed test function. The main result of the paper, the form of Q_C, is given at the end of section 3 in formula (3.10). Section 4 is devoted to numerical experiments. First the asymptotic result of section 3 is verified. This result states only the weak convergence of Q to Q_C and not the convergence of the solution f of the Levinson equation to the solution of the corresponding transport equation containing Q_C. The approximation of the solution of the transport equation is verified numerically in section 4 as well. The numerical solution of the transport equation involving the operator Q_C in (1.3) is nontrivial because this equation is implicit. We propose a solution method which is amenable to particle discretizations.

2. Scaling. We start by bringing the Levinson equation (1.2) into an appropriate dimensionless form. Choosing scales p_0, t_0 for the momentum p and the time t, and rescaling S by s_0, we set

$$f(p,t) = \frac{1}{p_0^3} f_s(p_s, t_s), \quad S(p, p', t) = s_0 S_s(p_s, p_s', t_s),$$
$$\varepsilon(p) = \frac{p_0^2}{m_*} \varepsilon_s(p_s), \quad p_s = \frac{p}{p_0}, \quad t_s = \frac{t}{t_0},$$

where m_* denotes the effective electron mass, and we obtain

$$\begin{aligned}
&\text{(a)}\quad \partial_{t_s} f_s(p_s,t_s) = s_0 t_0^2 p_0^3 \int_0^{t_s} dt'_s \int dp'_s [S_s(p_s,p'_s,t_s-t'_s) f_s(p'_s,t'_s) \\
&\qquad\qquad - S_s(p'_s,p_s,t_s-t'_s) f_s(p_s,t'_s)], \\
&\text{(b)}\quad S_s(p_s,p'_s,t_s) = \frac{2VF^2 n}{s_0(2\pi\hbar)^3} \cos\left[\frac{t_0 p_0^2 t_s}{m_*\hbar}\left(\varepsilon_s(p_s)-\varepsilon_s(p'_s)-\frac{m_*\hbar\omega}{p_0^2}\right)\right] \\
&\qquad + \frac{2VF^2(n+1)}{s_0(2\pi\hbar)^3} \cos\left[\frac{t_0 p_0^2 t_s}{m_*\hbar}\left(\varepsilon_s(p_s)-\varepsilon_s(p'_s)+\frac{m_*\hbar\omega}{p_0^2}\right)\right],
\end{aligned} \tag{2.1}$$

where, in the case of parabolic bands, $\varepsilon_s(p_s) = \frac{|p_s|^2}{2}$ holds. For the rest of this paper we will restrict ourselves to parabolic bands and assume that the matrix element F of the electron-phonon interaction is constant with respect to momentum.

The parameter s_0 can be chosen more or less freely, since it cancels as soon as (2.1)(b) is inserted into (2.1)(a). We choose $s_0 = \frac{1}{t_0^2 p_0^3}$, which ensures that the resulting equation varies on an $O(1)$ scale in time. The key issue is now to choose an appropriate scale p_0 for the momentum variable. A natural choice is to scale the phonon energy to unity, which gives $p_0^2 = m_*\hbar\omega$. Furthermore, we will consider the Levinson equation on a timescale that is much larger than the timescale on which the lattice vibrates. Therefore we set $t_0 = (\lambda\omega)^{-1}$, where λ denotes a dimensionless parameter. We drop the subscript s from here on and obtain

$$\begin{aligned}
\partial_t f(p,t) &= \int_0^t dt' \int dp' [S(p,p',t-t') f(p',t') - S(p',p,t-t') f(p,t')], \\
S(p,p',t) &= \frac{2VF^2}{\lambda^2(2\pi)^3}\sqrt{\frac{m_*^3}{\hbar^3\omega}}\left(n\cos\left[\frac{t}{\lambda}(\varepsilon(p)-\varepsilon(p')-1)\right]\right. \\
&\qquad \left. + (n+1)\cos\left[\frac{t}{\lambda}(\varepsilon(p)-\varepsilon_s(p')+1)\right]\right).
\end{aligned}$$

Since the scattering rate varies on a timescale of order $\frac{1}{\lambda}$, the amplitude should be of the same order to keep the integral of order $O(1)$, which is obtained by setting

$$\lambda^2 = \frac{2VF^2(n+1)}{(2\pi)^3}\sqrt{\frac{m_*^3}{\hbar^3\omega}}. \tag{2.2}$$

This gives a scaled equation of the form

$$\begin{aligned}
&\text{(a)}\quad \partial_t f(p,t) = Q_\lambda[f](p,t) \\
&\qquad\qquad := \int_0^t dt' \int dp' [S_\lambda(p,p',t-t') f(p',t') - S_\lambda(p',p,t-t') f(p,t')], \\
&(b)\quad S_\lambda(p,p',t) = \sum_{\nu=\pm 1} \frac{a_\nu}{\lambda}\cos\left[\frac{t}{\lambda}(\varepsilon(p)-\varepsilon(p')+\nu)\right], \quad a_{-1} = \frac{n}{n+1}, \quad a_1 = 1.
\end{aligned} \tag{2.3}$$

Thus we consider an asymptotic regime where the quantity λ defined by (2.2) is small, and consider the asymptotic behavior of the collision operator in the Levinson equation for timescales $t_0 = (\lambda\omega)^{-1}$, which are much larger than the scale on which the lattice vibrates.

We conclude this section with the following observation, giving a heuristic argument for the convergence to the Fermi golden rule operator. Changing variables in the integral in (2.3)(a), we obtain

$$Q_\lambda[f](p,t) = \int_0^{t/\lambda} d\tau \int dp' [\lambda S_\lambda(p,p',\lambda\tau) f(p',t-\lambda\tau) - \lambda S_\lambda(p',p,\lambda\tau) f(p,t-\lambda\tau)],$$
$$\lambda S_\lambda(p,p',\lambda\tau) = \sum_{\nu=\pm 1} a_\nu \cos[\tau(\varepsilon(p) - \varepsilon(p') + \nu)].$$

If the term $\lambda S_\lambda(p,p',\lambda\tau)$, which is actually independent of λ, would decay for large τ, we could Taylor-expand the solution f and obtain in zeroth order

$$\partial_t f(p,t) = \int_0^\infty d\tau \int dp' [\lambda S(p,p',\lambda\tau) f(p',t) - \lambda S(p',p,\lambda\tau) f(p,t)],$$

which makes the collision operator local in time. The corresponding scattering rate would then be given by

$$\int_0^\infty \lambda S(p,p',\lambda\tau) d\tau = \sum_{\nu=\pm 1} a_\nu \int_0^\infty \cos[\tau(\varepsilon(p) - \varepsilon(p') + \nu)] d\tau,$$

and the integral over the cosine produces the δ-function in the Fermi golden rule. This heuristic argument has been given in [1], [3], [5]. Although S does not decay for large times, this result still holds, but the limit process is oscillatory; i.e., we have to compute a weak limit for $\lambda \to 0$. The computation of this weak limit is the subject of the present paper.

3. Asymptotics. In this section we derive the asymptotic behavior of the collision operator Q_λ in (2.3) for $\lambda \to 0$ and show that Q_λ indeed converges to the Fermi golden rule operator in the weak sense. More importantly, we are able to derive the first order term in the asymptotic expansion. This enables us to obtain a corrected Fermi golden rule operator which is still local in time, and thus a corrected Boltzmann equation which better reflects the effects of finite collision times. The main result of this section is stated in Theorem 3.2, which gives an asymptotic expression for the Levinson operator Q_λ in (2.3) up to terms of order $o(\lambda)$ in the weak sense. This approximation is still local in time in the sense that it depends only on the values of the density function f at time t and on its time derivative. The first order approximation is, although local in time, only given in a weak sense in p since the scattering rates in the loss term will contain integrals which exist only as principal value. The form of the resulting approximate collision operator is given in formulas (3.7) and (3.10).

Since we are considering a weak limit, we will define, for a given density f, the functional

$$Y_\lambda(f,\psi) = \int_0^\infty dt \int dp \psi(p,t) Q_\lambda[f](p,t)$$

for a smooth test function ψ, and investigate the limiting behavior of $Y_\lambda(f,\psi)$ for $\lambda \to 0$. It will be convenient to rewrite Y_λ using the adjoint of the collision operator. Interchanging the integration variables p and p' in the first part of (2.3)(a) gives

$$\text{(3.1)} \quad \begin{aligned} &\text{(a)} \quad Y_\lambda(f,\psi) = \int_0^\infty dt \int dp [f(p,t) Q_\lambda^{adj}[\psi](p,t)], \\ &\text{(b)} \quad Q_\lambda^{adj}[\psi](p,t) = \int_t^\infty dt' \int dp' [S_\lambda(p',p,t'-t)(\psi(p',t') - \psi(p,t'))], \end{aligned}$$

where we have also interchanged the time variables t, t'. In this form it is easy to see that the collision operator Q_λ conserves mass locally in time since the adjoint operator $Q_\lambda^{adj}(\psi)$ equals zero for test functions ψ which are constant in the momentum direction. The functional Y_λ represents a convolution in time and is therefore best expressed through Fourier transforms. To this end, we extend the definition (3.1)(b) of the adjoint collision operator $Q_\lambda^{adj}[\psi](p,t)$ for negative time. We define the Fourier transforms of the truncated density function f and the test functions by

$$\hat{f}(p,\tau) = \frac{1}{\sqrt{2\pi}} \int dt[H(t)f(p,t)e^{-i\tau t}], \qquad \hat{\psi}(p,\tau) = \frac{1}{\sqrt{2\pi}} \int dt[\psi(p,t)e^{-i\tau t}], \tag{3.2}$$

where $H(t)$ denotes the Heaviside function. From now on all integrals are to be understood as being over the whole real line or all of $\mathbb{R}^3$ unless stated explicitly otherwise. We have the following.

PROPOSITION 3.1. *In terms of the Fourier transform of the truncated density function f and the test function ψ, the functional $Y_\lambda(f,\psi)$ is given by*

$$\text{(a)} \quad Y_\lambda(f,\psi) = \int dp \int d\tau \{\hat{f}^*(p,\tau)\hat{Q}_\lambda^{adj}[\psi](p,\tau)\},$$

$$\text{(b)} \quad \hat{Q}_\lambda^{adj}[\psi](p,\tau) = \frac{1}{2} \sum_{\nu,\sigma=\pm 1} a_\nu \int dp' \left[\frac{\pi}{\lambda} \delta\left(\frac{\sigma}{\lambda} w_\nu(p',p) - \tau \right) + \frac{1}{i(\sigma w_\nu(p',p) - \lambda\tau)} \right] [\hat{\psi}(p',\tau) - \hat{\psi}(p,\tau)], \tag{3.3}$$

where * denotes the complex conjugate and $w_\nu(p',p) = \varepsilon(p') - \varepsilon(p) + \nu$ holds.

Proof of Proposition 3.1. If we define the Fourier transform of the adjoint operator $Q_\lambda^{adj}[\psi]$ by

$$\hat{Q}_\lambda^{adj}[\psi](p,\tau) = \frac{1}{\sqrt{2\pi}} \int dt \int dt' \int dp' H(t'-t) S_\lambda(p',p,t'-t)[\psi(p',t') - \psi(p,t')]e^{-i\tau t}, \tag{3.4}$$

the functional Y_λ becomes

$$Y_\lambda(f,\psi) = \int d\tau \int dp[\hat{f}^*(p,\tau)\hat{Q}^{adj}[\psi](p,\tau)],$$

where from here on * will denote the complex conjugate. In order to compute the Fourier transform of the adjoint collision operator Q^{adj}, we have to essentially compute the Fourier transform of the function $H(t)\cos(ut)$ as a distribution in t. We choose a sufficiently smooth test function $\phi(t)$, which is compactly supported in time, and compute the integral

$$\int dt[H(t)\cos(ut)\phi(t)].$$

We split the integrand into its even and odd parts by writing

$$\cos(ut)\phi(t) = a(u,t) + \partial_t b(u,t),$$

where a and b are both real and even functions in time. These functions are given by

$$a(u,t) = \frac{1}{2}\cos(ut) \sum_{\gamma=\pm 1} \phi(\gamma t), \qquad b(u,t) = -\frac{1}{2} \int_{|t|}^{\infty} ds \left[\cos(us) \sum_{\gamma=\pm 1} \gamma\phi(\gamma s) \right]$$

and are both compactly supported in time as well. Their Fourier transforms in time satisfy

$$\hat{a}(u,\tau) = \frac{1}{4}\sum_{\sigma,\gamma=\pm 1} \hat{p}hi(\gamma\tau - \sigma u), \qquad \hat{b}(u,\tau) = \frac{1}{4i\tau}\sum_{\sigma,\gamma=\pm 1} \gamma\hat{p}hi(\gamma\tau - \sigma u)$$

and are both well defined, also for $\tau \to 0$. Since both a and b are even functions of t, we can extend the integral now over the whole real line and write

$$\begin{aligned}\int dt[H(t)\cos(ut)\phi(t)] &= \int_0^\infty \cos(ut)\phi(t)dt = \frac{1}{2}\int a(u,t)dt - b(u,0)\\ &= \frac{\sqrt{2\pi}}{2}\hat{a}(u,0) - \frac{1}{\sqrt{2\pi}}\int \hat{b}(u,\tau)d\tau.\end{aligned}$$

Inserting the expressions for the Fourier transforms of a and b gives

$$\int dt[H(t)\cos(ut)\phi(t)] = \frac{1}{4\sqrt{2\pi}}\sum_{\sigma,\gamma=\pm 1}\left\{\pi\hat{p}hi(-\sigma u) - \int \frac{\gamma}{i\tau}\hat{p}hi(\gamma\tau - \sigma u)d\tau\right\}.$$

Shifting the integration variable in the second term gives, since the result does not depend on the summation index γ anymore,

$$\int dt[H(t)\cos(ut)\phi(t)] = \frac{1}{2\sqrt{2\pi}}\sum_{\sigma=\pm 1}\left\{\pi\hat{p}hi(-\sigma u) - \int \frac{\hat{p}hi(\tau)}{i(\tau+\sigma u)}d\tau\right\}.$$

Finally, we introduce a δ-function to have a more compact notation, obtaining that

$$\int dt[H(t)\cos(ut)\phi(t)] = \frac{1}{2\sqrt{2\pi}}\sum_{\sigma=\pm 1}\int\left[\pi\delta(\tau+\sigma u) - \frac{1}{i(\tau+\sigma u)}\right]\hat{p}hi(\tau)d\tau$$

holds for all test functions $\phi(t)$ which are compactly supported in t. Thus, in a weak sense, i.e., when integrated against the Fourier transform of compactly supported test functions,

$$[\widehat{H(t)\cos(ut)}](\tau) = \frac{1}{2\sqrt{2\pi}}\sum_{\sigma=\pm 1}\left[\pi\delta(\tau+\sigma u) + \frac{1}{i(\tau+\sigma u)}\right]$$

holds. Equipped with this, we can express the convolution integral for $\hat{Q}^{adj}$ in (3.4) as

$$\begin{aligned}\hat{Q}^{adj}[\psi](p,\tau) &= \sqrt{2\pi}\int dp'\{[H(t)\widehat{S_\lambda(p')},p,t)](-\tau)[\hat{\psi}(p',\tau) - \hat{\psi}(p,\tau)]\}\\ &= \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int dp'\left[\frac{\pi}{\lambda}\delta\left(\frac{\sigma}{\lambda}w_\nu(p',p) - \tau\right)\right.\\ &\qquad\left. + \frac{1}{i(\sigma w_\nu(p',p) - \lambda\tau)}\right][\hat{\psi}(p',\tau) - \hat{\psi}(p,\tau)],\\ w_\nu(p',p) &:= \varepsilon(p') - \varepsilon(p) + \nu. \qquad \square\end{aligned}$$

We now change to energy-angle variables. We make the coordinate transformation in momentum space of the form

$$p \to (\varepsilon(p), p_0), \quad p_0 := \frac{p}{|p|},$$

where p_0 is a vector living only on the unit sphere. Carrying out this coordinate transformation in integrals and directional derivatives in the radial direction for the parabolic band energy $\varepsilon(p) = \frac{|p|^2}{2}$, this means

$$\int f(p)dp = \int_0^\infty d\varepsilon \int dp_0 f(\varepsilon, p_0)\sqrt{2\varepsilon}, \quad \int 1 dp_0 = 4\pi, \quad p^T \nabla_p f(p) = 2\varepsilon \partial_\varepsilon f(\varepsilon, p_0),$$

and the functional $Y_\lambda(f, \psi)$ in (3.3) is given by

$$\text{(a)} \quad Y_\lambda(f,\psi) = \int_0^\infty d\varepsilon \int dp_0 \int d\tau \left\{ \sqrt{2\varepsilon} \hat{f}^*(\varepsilon, p_0, \tau) \hat{Q}_\lambda^{adj}[\psi](\varepsilon, p_0, \tau) \right\},$$

$$\begin{aligned} \text{(b)} \quad \hat{Q}_\lambda^{adj}[\psi](\varepsilon, p_0, \tau) = \frac{1}{2} \sum_{\nu,\sigma=\pm 1} a_\nu \int_0^\infty d\varepsilon' \int dp_0' \\ \times \sqrt{2\varepsilon'} \Bigg[\pi \delta(\varepsilon' - \varepsilon + \nu - \sigma\lambda\tau) \\ + \frac{\sigma}{i(\varepsilon' - \varepsilon + \nu - \sigma\lambda\tau)} \Bigg] [\hat{\psi}(\varepsilon', p_0', \tau) - \hat{\psi}(\varepsilon, p_0, \tau)], \end{aligned} \tag{3.5}$$

where we have made use of the identity $\frac{1}{\lambda}\delta(\frac{z}{\lambda}) = \delta(z)$ and the fact that the δ-function is even. We now give the weak expansion of the collision operator Q_λ as follows.

THEOREM 3.2. *For any fixed test function $\psi(\varepsilon, p_0, t)$ whose Fourier transform in time $\hat{\psi}(\varepsilon, p_0, \tau)$ decays sufficiently fast, the value of the functional $Y_\lambda(f, \psi)$ can be written as*

$$\text{(a)} \quad Y_\lambda(f,\psi) = Y_0(f,\psi) + \lambda Y_1(f,\psi) + o(\lambda), \tag{3.6}$$

with Y_0 and Y_1 given by

$$\begin{aligned} \text{(b)} \quad Y_0(f,\psi) = \sum_{\nu=\pm 1} a_\nu \int_0^\infty d\varepsilon \int dp_0 \int_0^\infty d\varepsilon' \int dp_0' \int_0^\infty dt \\ \pi \delta(\varepsilon' - \varepsilon + \nu) \sqrt{2\varepsilon'}\sqrt{2\varepsilon} f(\varepsilon, p_0, t)[\psi(\varepsilon', p_0', t) - \psi(\varepsilon, p_0, t)], \end{aligned}$$

$$\begin{aligned} \text{(c)} \quad Y_1(f,\psi) = -\sum_{\nu=\pm 1} a_\nu \int_0^\infty d\varepsilon \int dp_0 \int_0^\infty d\varepsilon' \int dp_0' \int_0^\infty dt \\ \ln(|\varepsilon' - \varepsilon + \nu|) \partial_{\varepsilon'} \partial_\varepsilon \left(\sqrt{2\varepsilon'}\sqrt{2\varepsilon} f(\varepsilon, p_0, t) \partial_t [\psi(\varepsilon', p_0', t) - \psi(\varepsilon, p_0, t)] \right). \end{aligned}$$

The proof of Theorem 3.2 is deferred to the end of this section.

Remark: In the usual Cartesian coordinates this means that the collision operator Q_λ is given in weak form by

$$\text{(a)} \quad Q_\lambda[f] = Q_0[f] + \lambda Q_1[f] + o(\lambda), \tag{3.7}$$

$$\text{(b)} \quad Q_0[f](p,t) = \sum_{\nu=\pm 1} \pi a_\nu \int dp' [\delta(\varepsilon - \varepsilon' + \nu) f(p', t) - \delta(\varepsilon' - \varepsilon + \nu) f(p, t)],$$

$$\begin{aligned} \text{(c)} \quad \int dp [\phi(p) Q_1[f](p,t)] = \sum_{\nu=\pm 1} a_\nu \int dp \int dp' \\ \ln(|\varepsilon' - \varepsilon + \nu|) \frac{1}{4\varepsilon\varepsilon'} (p^T \nabla p)((p')^T \nabla_{p'}) \left[\sqrt{4\varepsilon\varepsilon'} \partial_t f(p,t)(\phi(p') - \phi(p)) \right], \end{aligned}$$

where the first order term Q_1 is formulated weakly in the momentum direction only, in order to guarantee that the integrals converge. What remains of the nonlocality in time of the Levinson operator Q_λ in (2.3) is that the operator Q_1 in (3.7)(c) acts on the time derivative of the density function f.

Remark: Theorem 3.2 states only the weak convergence of the Levinson operator (1.2) towards the Fermi golden rule operator (1.1)(b) and not the convergence of solutions of the Levinson equation towards solutions of the corresponding Boltzmann equation. Since solutions of the Boltzmann equation remain nonnegative for nonnegative initial data, a weak convergence result for solutions would actually imply that the Wigner function and its density matrix equivalent would remain nonnegative definite for all time.

Note that Theorem 3.2 holds only for a fixed function f which is independent of λ. However, its validity can be extended by considering a filtered collision operator, since convolution integrals are commutative. If we choose a test function ψ which is of the form $\psi(p,t) = \phi(p)\Gamma(s-t)$ for any s, whose Fourier transform is given by $\hat{\psi}(p,\tau) = \phi(p)\hat{\Gamma}(\tau)^* e^{i\tau s}$, then the Fourier transform of the convolution kernel can be transferred onto the Fourier transform of f, and (3.3)(a) reads

$$Y_\lambda(f_\lambda,\psi) = \sqrt{2\pi}\int dp \int d\tau\{\hat{f}^*_\lambda(p,\tau)\hat{\Gamma}^*(\tau)\hat{Q}^{adj}_\lambda[\phi(p)\delta(t-s)](p,\tau)\}.$$

Theorem 3.2 will still hold as long as the function $\hat{f}^*_\lambda(p,\tau)\hat{\Gamma}(\tau)$ decays sufficiently fast in the variable τ. This means that, even for a function which is oscillating rapidly in time, the filtered operator

$$Q^F_\lambda[f_\lambda](p,t) = \int \Gamma(t-s)Q_\lambda[f_\lambda](p,s)ds \tag{3.8}$$

will satisfy

$$Q^F_\lambda[f_\lambda] = Q_0[f^F_\lambda] + \lambda Q_1[f^F_\lambda] + o(\lambda) \tag{3.9}$$

pointwise in t, where the filtered signal $f^F_\lambda(p,t)$ is given by

$$\hat{f}^F_\lambda(p,\tau) = \sqrt{2\pi}\hat{\Gamma}(\tau)\hat{f}_\lambda(p,\tau), \qquad f^F_\lambda(p,t) = \int \Gamma(t-s)H(s)f_\lambda(p,s)ds.$$

The unscaled equation. Finally, we reverse the scaling of section 2 and write the corrected Fermi golden rule in dimensional variables. Undoing the scaling and choosing the strong form gives the following corrected Boltzmann equation:

$$\partial_t f(p,t) = \int dp' S_0(p,p')f(p',t) - \kappa_0(p)f(p,t) + \int dp' S_1(p,p')\partial_t f(p',t) - \partial_t\kappa_1(p)f(p,t). \tag{3.10}$$

The transition rates S_j and the out-scattering rates κ_j are

$$S_0(p,p') = \frac{V}{(2\pi\hbar)^3}\sum_{\nu=\pm1}\frac{2\pi}{\hbar}M^2\left(n+\frac{1}{2}+\frac{\nu}{2}\right)\delta(\varepsilon(p)-\varepsilon(p')+\nu\hbar\omega),$$

$$S_1(p,p') = \frac{V}{(2\pi\hbar)^3}\sum_{\nu=\pm1}2M^2\left(n+\frac{1}{2}+\frac{\nu}{2}\right)\frac{1}{(\varepsilon(p)-\varepsilon(p')+\nu\hbar\omega)^2},$$

$$\kappa_j(p) = \int dp' S_j(p',p), \quad j=0,1,$$

where $M = \hbar F$ holds, and it should again be pointed out that the strong form of the collision operator is purely formal; i.e., the integral in the out-scattering rate κ_1 is actually infinite, and the first order term has to be formulated in the weak form (3.7).

We conclude this section with the proof of Theorem 3.2.

Proof of Theorem 3.2. We start by writing (3.5) in a more compact form as

(3.11)
$$Y_\lambda(f,\psi) = \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau A_\sigma'(\varepsilon' - \varepsilon + \nu - \sigma\lambda\tau) B(\varepsilon,\varepsilon',p_0,p_0',\tau)\sqrt{2\varepsilon'}^{+},$$

where we have formally extended the integrals with respect to the energy variables ε, ε' over the whole real line and denote by $\sqrt{z}^{+}$ the truncated root; i.e., $\sqrt{z}^{+} = 0$ for $z < 0$ holds. This notation will simplify the further derivation. Here the function $A(u)$, its derivative $A'(u)$, and B are given by

(3.12)
$$\text{(a)}\quad A_\sigma(u) = \pi H(u) - i\sigma \ln(|u|), \qquad A_\sigma'(u) = \pi\delta(u) - \frac{i\sigma}{u},$$
$$\text{(b)}\quad B(\varepsilon,\varepsilon',p_0,p_0',\tau) = \sqrt{2\varepsilon}^{+}\hat{f}^{*}(\varepsilon,p_0,\tau)[\hat{\psi}(\varepsilon',p_0',\tau) - \hat{\psi}(\varepsilon,p_0,\tau)].$$

Shifting the ε' variable in (3.11) gives

$$Y_\lambda(f,\psi) = \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau A_\sigma'(\varepsilon' - \varepsilon + \nu) B(\varepsilon,\varepsilon' + \sigma\lambda\tau,p_0,p_0',\tau)\sqrt{2(\varepsilon' + \sigma\lambda\tau)}^{+}.$$

In principle, we are now going to Taylor-expand the function B with respect to the variable ε'. This is admissible since the variable ε' only appears in the argument of the test function $\hat{\psi}$ in the definition of B, and therefore the function $\partial_{\varepsilon'}B$ decays sufficiently fast in ε' as well. However, care has to be taken with the various singularities appearing in the integrals. We remove the singularity in the function A_σ' by integrating by parts with respect to ε and obtain

$$Y_\lambda(f,\psi) = \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau \; A_\sigma(\varepsilon' - \varepsilon + \nu)\partial_\varepsilon B(\varepsilon,\varepsilon' + \sigma\lambda\tau,p_0,p_0',\tau)\sqrt{2(\varepsilon' + \sigma\lambda\tau)}^{+}.$$

Now we Taylor-expand the function B with respect to the variable ε' and write

(3.13)
$$\partial_\varepsilon B(\varepsilon,\varepsilon' + \sigma\lambda\tau,p_0,p_0',\tau) = \partial_\varepsilon B(\varepsilon,\varepsilon',p_0,p_0',\tau) + \sigma\lambda\tau\partial_\varepsilon\partial_{\varepsilon'}B(\varepsilon,\varepsilon',p_0,p_0',\tau) + O(\lambda^2).$$

This is admissible since the function B is compactly supported in the variable ε'. Next we formally expand the volume element $\sqrt{2\varepsilon'}^{+}$ and write

$$\sqrt{2(\varepsilon' + \sigma\lambda\tau)}^{+} = \sqrt{2\varepsilon'}^{+} + \frac{\sigma\lambda\tau H(\varepsilon')}{\sqrt{2\varepsilon'}} + \frac{\lambda\sigma\tau}{(\varepsilon')^{\alpha}}R_\alpha(\varepsilon',\lambda\sigma\tau) \tag{3.14}$$

for some α, which of course is, at this point, only a definition for the remainder term R_α. Inserting (3.13) and (3.14) into the definition for $Y_\lambda(f,\psi)$, and neglecting the $O(\lambda^2)$ terms in (3.13), gives

$$Y_\lambda = Y_0 + \lambda Y_1 + \lambda Y_{2\lambda} + O(\lambda^2)$$

with

$$\begin{aligned}
&Y_0(f,\psi)\\
&= \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau A'_\sigma(\varepsilon'-\varepsilon+\nu)\sqrt{2\varepsilon'}^{+} B(\varepsilon,\varepsilon',p_0,p_0',\tau),\\
&Y_1(f,\psi)\\
&= \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau A_\sigma(\varepsilon'-\varepsilon+\nu)\sigma\tau\partial_{\varepsilon'}\partial_\varepsilon(\sqrt{2\varepsilon'}^{+} B(\varepsilon,\varepsilon',p_0,p_0',\tau)),\\
&Y_{2\lambda}(f,\psi)\\
&= \frac{1}{2}\sum_{\nu,\sigma=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau A_\sigma(\varepsilon'-\varepsilon+\nu)\frac{\sigma\tau}{(\varepsilon')^\alpha}\\
&\qquad \times \partial_\varepsilon B(\varepsilon,\varepsilon'+\sigma\lambda\tau,p_0,p_0',\tau)R_\alpha(\varepsilon',\lambda\sigma\tau).
\end{aligned}$$

Inserting the definition of the function A_σ from (3.12), we see that odd terms in σ will cancel in Y_0, and the even terms in σ will cancel in Y_1, giving

$$\begin{aligned}
&Y_0(f,\psi)\\
&= \sum_{\nu=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau\pi\delta(\varepsilon'-\varepsilon+\nu)\sqrt{2\varepsilon'}^{+} B(\varepsilon,\varepsilon',p_0,p_0',\tau),\\
&Y_1(f,\psi)\\
&= -\sum_{\nu=\pm 1} a_\nu \int d\varepsilon \int dp_0 \int d\varepsilon' \int dp_0' \int d\tau \ln(|\varepsilon'-\varepsilon+\nu|)i\tau\partial_{\varepsilon'}\partial_\varepsilon\left(\sqrt{2\varepsilon'}^{+} B(\varepsilon,\varepsilon',p_0,p_0',\tau)\right).
\end{aligned}$$

Reversing the Fourier transforms in time gives (3.6)(b,c). The term Y_0 produces the Fermi golden rule, and the term Y_1 the $O(\lambda)$ correction to it. It remains to estimate the term $Y_{2\lambda}$. Since the singularity in the integrand A_σ in ε' is only logarithmic, the integrals will converge for $\alpha < 1$. It therefore remains to choose α such that R_α remains uniformly bounded in ε'; i.e., we can write

(3.15)
$$|Y_{2\lambda}(f,\psi)| \le const \max\{|R_\alpha(\varepsilon',\lambda\sigma\tau)|,\ 0\le\varepsilon'<\infty,\ |\tau|\le K\} \quad \text{for } 0<\alpha<1,$$

where we only have to consider a finite range for τ, since the test function $\hat{\psi}$ can be assumed to be compactly supported. Thus we have to estimate the term

$$\max\{|R_\alpha(\varepsilon',z)|,\ 0\le\varepsilon'<\infty,\ |z|\le\lambda K\}.$$

According to (3.14), R_α is given by

$$R_\alpha(\varepsilon',z) = (\varepsilon')^\alpha\left[\frac{\sqrt{2(\varepsilon'+z)}^{+}-\sqrt{2\varepsilon'}^{+}}{z} - \frac{H(\varepsilon')}{\sqrt{2\varepsilon'}}\right]$$

or

$$R_\alpha(\varepsilon', z) = \begin{pmatrix} (\varepsilon')^\alpha \left[\dfrac{-\sqrt{2\varepsilon'}}{z} - \dfrac{1}{\sqrt{2\varepsilon'}} \right] & \text{for } 0 \le \varepsilon' \le \max\{-z, 0\} \\ (\varepsilon')^\alpha \left[\dfrac{\sqrt{2(\varepsilon'+z)} - \sqrt{2\varepsilon'}}{z} - \dfrac{1}{\sqrt{2\varepsilon'}} \right] & \text{for } \max\{-z, 0\} \le \varepsilon' \end{pmatrix}, \tag{3.16}$$

where the first row is relevant only for $z < 0$. If we choose $\alpha > \frac{1}{2}$, then we can estimate

$$(\varepsilon')^\alpha \left| \frac{-\sqrt{2\varepsilon'}}{z} - \frac{1}{\sqrt{2\varepsilon'}} \right| \le \sqrt{2}(-z)^{\alpha-1/2} + \frac{1}{\sqrt{2}}(-z)^{\alpha-1/2} = O(\lambda^{\alpha-1/2}) \quad \text{for } 0 \le \varepsilon' \le -z,$$

which takes care of the first row of (3.16). To estimate the second row of (3.16), we rewrite the expression as

$$\begin{aligned} &\left| (\varepsilon')^\alpha \left[\frac{\sqrt{2(\varepsilon'+z)} - \sqrt{2\varepsilon'}}{z} - \frac{1}{\sqrt{2\varepsilon'}} \right] \right| \\ &\quad = \frac{(\varepsilon')^\alpha}{\sqrt{2\varepsilon'}} \left| \frac{1 - \sqrt{1+\frac{z}{\varepsilon'}}}{1+\sqrt{1+\frac{z}{\varepsilon'}}} \right| = \frac{|z|^{\alpha-1/2}}{\sqrt{2}} \left| \frac{z}{\varepsilon'} \right|^{1/2-\alpha} \left| \frac{1 - \sqrt{1+\frac{z}{\varepsilon'}}}{1+\sqrt{1+\frac{z}{\varepsilon'}}} \right| \\ &\quad \le \frac{|z|^{\alpha-1/2}}{\sqrt{2}} \max_{-1 \le x < \infty} \left\{ |x|^{1/2-\alpha} \left| \frac{1-\sqrt{1+x}}{1+\sqrt{1+x}} \right| \right\} = O(\lambda^{\alpha-1/2}) \quad \text{for } \alpha > \frac{1}{2}. \end{aligned}$$

Thus, in summary, $\max\{|R_\alpha(\varepsilon', \lambda\sigma\tau)|, 0 \le \varepsilon' \le K, |\tau| \le K\} = O(\lambda^{\alpha-1/2})$ will hold for any $\alpha > \frac{1}{2}$, and because of (3.15), $Y_{2\lambda}(f, \psi) = O(\lambda^{\alpha-1/2})$ will hold for any $\frac{1}{2} < \alpha < 1$. Therefore $\lambda Y_{2\lambda}$ is actually a term of order $o(\lambda)$, although not of order $O(\lambda^2)$, and can be neglected in the first order approximation. Inserting the definition (3.12)(b) for the function B into Y_0, Y_1 and reversing the Fourier transforms gives the result. ∎

4. Numerical results. In this section we verify the asymptotic analysis of the previous section numerically. This verification will consist of two parts. The first part is concerned directly with the weak approximation of the operator Q_λ by $Q_0 + \lambda Q_1$, i.e., with the verification of Theorem 3.2. The more interesting question is of course in what sense the solution of the zero field Levinson equation (1.2) is approximated by the solution of the corresponding approximate equation. To answer this question rigorously we would need some form of stability or entropy estimate for the Levinson equation (1.2). This will be the subject of future work. Nevertheless, the second part of this section is devoted to a numerical study of this question, i.e., a numerical comparison of the solution of the Levinson equation to the solution of an appropriate approximate problem based on the result in Theorem 3.2.

Discretization of the collision operators. For reasons of computational simplicity, we choose a finite difference discretization of the involved collision operators Q_0, Q_1, and Q_λ. While the discretization of the full collision operator Q_λ in (2.3) and the zero order term Q_0 in (3.7)(b) (the Fermi golden rule) by finite differences is straightforward, some care has to be taken when discretizing the first order term Q_1 in (3.7)(c), since it is only formulated in a weak sense. This means that the corresponding strong formulation of the operator Q_1 will contain diverging integrals.

Integrating (3.6)(c) by parts to obtain the strong version of Q_1 gives

$$Q_1[f](p,t) = \int dp'[S_1(p,p')\partial_t f(p',t) - S_1(p',p)\partial_t f(p,t)]$$

with the first order scattering cross section S_1 given by

$$S_1(p,p') = \sum_{\nu=\pm 1} \frac{a_\nu}{(\varepsilon(p) - \varepsilon(p') + \nu)^2}, \tag{4.1}$$

and the resulting integral will be infinite in the strong formulation. We therefore discretize the first order operator Q_1 in a weak difference form. We start by choosing a mesh in energy and time direction of the form

$$M_\varepsilon = \{\varepsilon : \varepsilon = j\Delta\varepsilon,\ j = 0,1,\dots\}, \quad \Delta\varepsilon = \frac{1}{K}, \qquad M_t = \{t : t = n\Delta t,\ n = 0,1,\dots\},$$

where we choose $\Delta\varepsilon$ conveniently in such a way that the emission/absorption energy, which is equal to unity in our scaling, is an integer multiple of the mesh size. The density function f can be assumed to be a function of the energy only, so $f = f(\varepsilon,t)$ holds. Using parabolic bands ($\varepsilon = \frac{|p|^2}{2}$), integrals with respect to the momentum p are approximated by

$$\int f(p,t)dp \approx \Delta\varepsilon \sum_{j=0}^{\infty} f(j\Delta\varepsilon,t)dp(j\Delta\varepsilon), \quad dp(\varepsilon) := 4\pi\sqrt{2\varepsilon}.$$

The full collision operator Q_λ in (2.3) is now approximated by

$$\begin{aligned} Q_\lambda[f](j\Delta\varepsilon, n\Delta t) := \Delta t\Delta\varepsilon \sum_{n'=0}^{n}\sum_{j'=0}^{\infty} dp(j'\Delta\varepsilon) \\ \times[S_\lambda(j\Delta\varepsilon, j'\Delta\varepsilon, (n-n')\Delta t)f(j'\Delta\varepsilon, n'\Delta t) \\ - S_\lambda(j'\Delta\varepsilon, j\Delta\varepsilon, (n-n')\Delta t)f(j\Delta\varepsilon, n'\Delta t)] \end{aligned}$$

with S_λ given as in (2.3)(c). The Fermi golden rule operator Q_0 is discretized by

$$Q_0[f](j\Delta\varepsilon,t) = \sum_{\nu=\pm 1} \pi a_\nu[dp((j+\nu K)\Delta\varepsilon)f((j+\nu K)\Delta\varepsilon,t) - dp((j-\nu K)\Delta\varepsilon)f(j\Delta\varepsilon,t)], \tag{4.2}$$

where, for notational simplicity, we simply set $dp(\varepsilon) = 0$ for $\varepsilon < 0$. The first order collision operator Q_1 in (3.7)(c) is given in its weak formulation by

$$\begin{aligned} \int dp(\varepsilon)[\phi(\varepsilon)Q_1[f](\varepsilon,t)]d\varepsilon = 16\pi^2 \sum_{\nu=\pm 1} a_\nu \int d\varepsilon \int d\varepsilon' \\ \times \ln(|\varepsilon' - \varepsilon + \nu|)\partial_\varepsilon\partial_{\varepsilon'}\left[\sqrt{4\varepsilon\varepsilon'}\partial_t f(\varepsilon,t)(\phi(\varepsilon') - \phi(\varepsilon))\right]. \end{aligned}$$

In this weak formulation the integrals are guaranteed to converge. It is therefore allowed to truncate the logarithmic singularity in the integral kernel. We define

$$\ln^0(j\Delta\varepsilon) = \begin{cases} \ln(j\Delta\varepsilon), & j > 0, \\ \ln(\Delta\varepsilon), & j = 0, \end{cases}$$

and discretize Q_1 in a weak finite difference sense by requiring that

$$\begin{aligned}\Delta\varepsilon \sum_{j=0}^{\infty} dp(j\Delta\varepsilon)[\phi(j\Delta\varepsilon)Q_1[f](j\Delta\varepsilon, n\Delta t)] \\ = 16\pi^2(\Delta\varepsilon)^2 \sum_{\nu=\pm 1} a_\nu \sum_{j=0}^{\infty}\sum_{j'=0}^{\infty} \\ \ln^0(|j'-j+\nu K|\Delta\varepsilon) D_j^+ D_{j'}^+ \left[\sqrt{4jj'}\Delta\varepsilon D_n^+ f(j\Delta\varepsilon, n\Delta t)(\phi(j'\Delta\varepsilon)-\phi(j\Delta\varepsilon))\right]\end{aligned}$$

hold for all grid-test-functions ϕ. Here D^+ denotes the usual forward difference operators acting on the respective indices; i.e.,

$$\begin{aligned}&\text{(a)} \quad D_j^+ f(j\Delta\varepsilon, t) = \frac{f((j+1)\Delta\varepsilon, t) - f(j\Delta\varepsilon, t)}{\Delta\varepsilon}, \\ &\text{(b)} \quad D_n^+ f(\varepsilon, n\Delta t) = \frac{f(\varepsilon, (n+1)\Delta t) - f(\varepsilon, n\Delta t)}{\Delta t},\end{aligned} \tag{4.3}$$

holds. Expressing the first order collision operator in a strong form on the discrete level, i.e., choosing a discrete δ-function for the test function ϕ, gives

(4.4)
$$\begin{aligned}&Q_1[f](j\Delta\varepsilon, n\Delta t) \\ &= \Delta\varepsilon \sum_{j'=0}^{\infty} dp(j\Delta\varepsilon)[S_1(j\Delta\varepsilon, j'\Delta\varepsilon) D_n^+ f(j'\Delta\varepsilon, n\Delta t) - S_1(j'\Delta\varepsilon, j\Delta\varepsilon) D_n^+ f(j\Delta\varepsilon, n\Delta t)],\end{aligned}$$

with the discrete scattering cross section S_1 given by

$$S_1(j\Delta\varepsilon, j'\Delta\varepsilon) = \sum_{\nu=\pm 1} a_\nu D_j^- D_{j'}^- \ln^0 |(j-j'+\nu K)\Delta\varepsilon|,$$

which is the appropriate approximation to the singular integral kernel (4.1). Here D^- denotes the backward differencing operator, analogously to the definition of D^+ in (4.3).

We now proceed to verify Theorem 3.2 numerically. Besides the verification of the asymptotic analysis of the previous section, the purpose of this exercise is also to gain some confidence in the weak difference discretization before computing asymptotic solutions to the Levinson equation. More precisely, we will verify the consequence of Theorem 3.2 given in (3.9), namely that the smoothed version of the full collision operator Q_λ applied to a highly oscillatory function is approximated by the zero- and first order terms Q_0 and Q_1 applied to the smoothed function. Figure 1 shows the signal chosen for this verification, which consists of the function $f(\varepsilon, t) = (1 + \cos(20t))/(1 + 3\varepsilon^2)$, i.e., a smooth function of ε modulated by a rapid oscillation in time. Figure 2 shows the filtered signal $f^F(\varepsilon, t)$, obtained by convoluting f with a Gaussian in time. We now compute $Q_\lambda[f]$ and the corresponding smoothed version $Q_\lambda^F[f]$ according to (3.8) and compare the result to $(Q_0 + \lambda Q_1)[f^F]$. As a measure for the approximation we chose the energy given by the formula

$$\langle \varepsilon Q \rangle(t) = \Delta\varepsilon \sum_{j=0}^{\infty} dp(j\Delta\varepsilon) j\Delta\varepsilon Q(j\Delta\varepsilon, t).$$

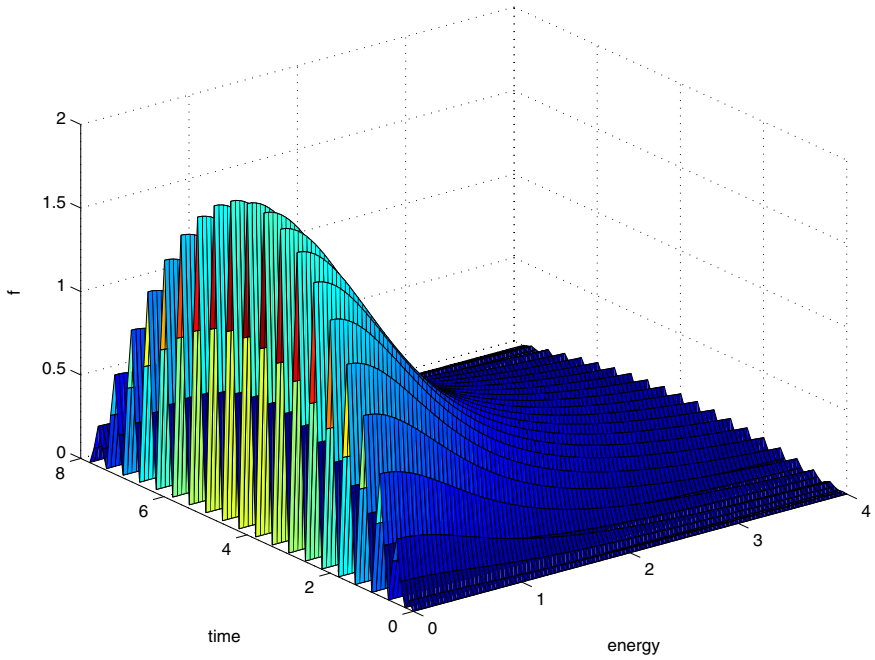

FIG. 1. *Unfiltered signal.*

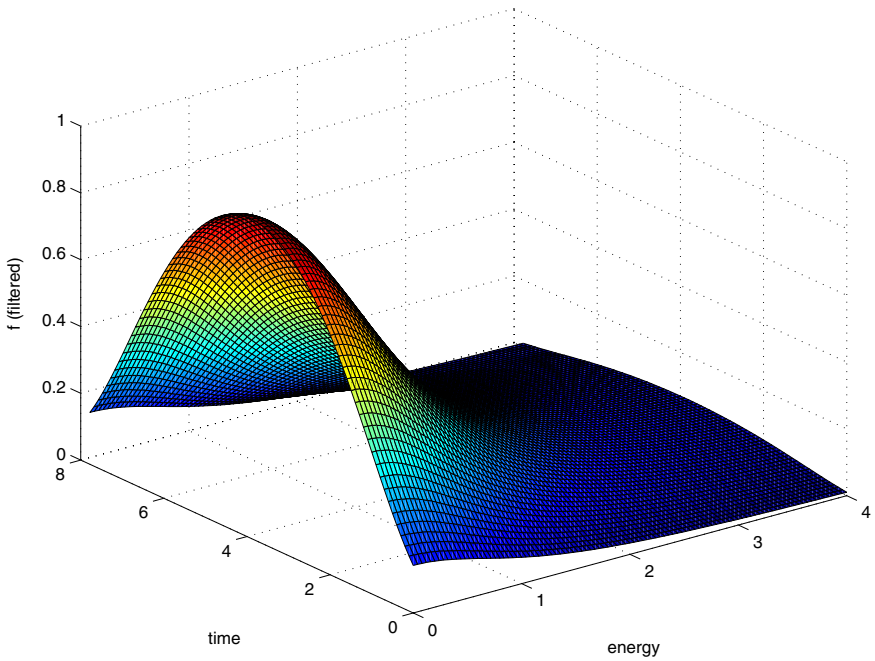

FIG. 2. *Filtered signal.*

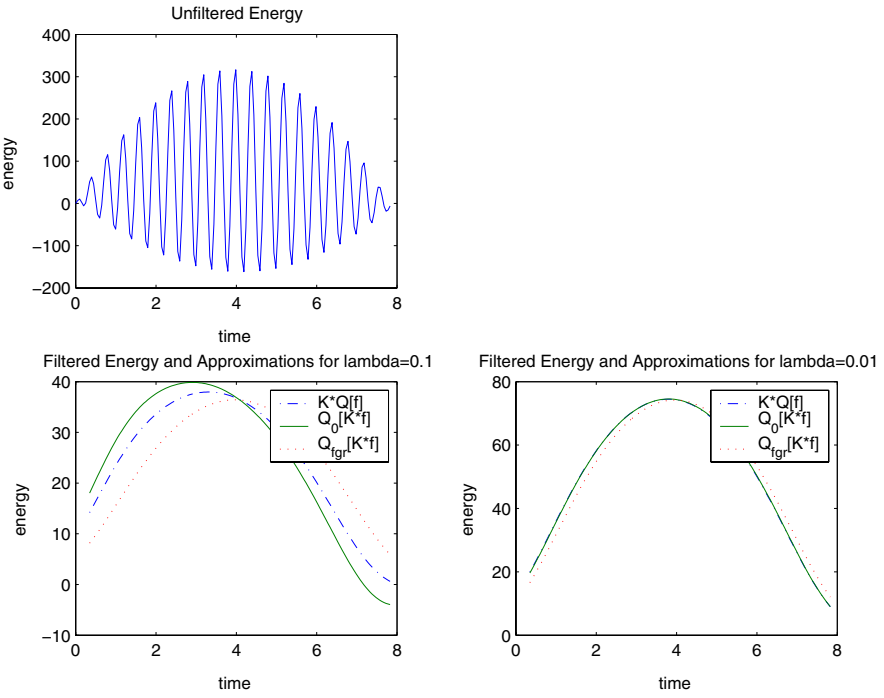

FIG. 3. *Comparison of energies.*

Figure 3 shows the highly oscillatory energy $\langle \varepsilon Q_\lambda[f] \rangle$ and compares $\langle \varepsilon Q_\lambda^F[f] \rangle$ to the values of $\langle \varepsilon Q_0[f^F] \rangle$ and $\langle \varepsilon (Q_0[f^F] + \lambda Q_1[f^F]) \rangle$ for $\lambda = 0.1$ and $\lambda = 0.01$. Figure 3 first confirms that the smoothed collision operator converges to the Fermi golden rule applied to the smoothed signal pointwise in time and that the approximation is improved by adding the first order correction, which is a direct consequence of the weak convergence given in Theorem 3.2.

We now turn to the more interesting question of whether, and in what sense, the solution of the zero field Levinson equation (1.2) is approximated by the solution of the asymptotic equation

$$\partial_t f = Q_0[f] + \lambda Q_1[f]. \tag{4.5}$$

To this end, we will compute with more realistic parameters. F in (1.2)(b) denotes the frequency of a particular lattice state and is given by the formula

$$F(\xi) = \sqrt{\frac{q^2 \hbar \omega}{2V|\xi|^2 \varepsilon_0} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s} \right)}, \tag{4.6}$$

where ξ is the momentum vector corresponding to the lattice state, ε_0 is the dielectricity constant (for vacuum), and ε_∞ and ε_s are the usual corrections to ε_0, taking into account the property of the crystal. The values for the physical parameters in

section 1 are summarized in the table below:

Symbol	Value	Unit	Meaning
q	$1.602 * 10^{-19}$	C	Electron charge
$\hbar$	$1.054 * 10^{-34}$	$\mathrm{kgm}^2/\mathrm{sec}$	Planck constant
h	$6.626196 * 10^{-34}$	$\mathrm{kgm}^2/\mathrm{sec}$	$h = 2\pi\hbar$
m_*	$0.063 * 0.109 * 10^{-31}$	kg	Effective electron mass
$\hbar\omega$	0.036	eV	Emission/absorption energy
ε_0	$8.85 * 10^{-12}$	$\frac{C}{V\mathrm{m}}$	Dielectricity constant (vacuum)
ε_∞	10.92	1	
ε_s	12.9	1	

We are considering the system at room temperature; i.e., the inverse temperature β in section 2 has a value of $\beta = 40(eV)^{-1}$, which gives a value of $n = 0.3105$ for the occupation number n. We consider only a single lattice state corresponding to the lattice being in equilibrium; i.e., we choose $|\xi|^2 = \frac{m_*}{\beta}$. Using these values, one computes a value of $\lambda = 0.0113$ for the dimensionless parameter λ, which suggests that we are in the appropriate asymptotic regime.

The asymptotic solution of the Levinson equation. The solution of the asymptotic equation (4.5) is complicated by the following facts. First, the equation is implicit in time, since the first order perturbation operator Q_1 acts on the time derivative of the solution f. Second, the implicit term is nonlocal in the energy variable, and third, this nonlocal implicit integral term contains a singular kernel. These factors make the actual numerical solution of (4.5) highly nontrivial. One could, for instance, be tempted to replace the time derivative of the density function in Q_1 in first order by $Q_0[f]$ and solve the explicit equation

$$\partial_t f = Q_0[f] + \lambda \int dp[S_1(p,p')Q_0[f](p',t) - S_1(p',p)Q_0[f](p,t)] \tag{4.7}$$

instead. It is, however, relatively easy to see (and has been verified numerically) that (4.7) is ill posed. At the level of computational complexity considered in this paper it would be feasible to directly discretize (4.5) using an implicit time discretization. We would then have to consider the artificial numerical diffusion generated by implicit methods, which is a major factor since we want to compare asymptotic solutions to the highly oscillatory solution of the Levinson equation. It should be pointed out here that we have made life particularly simple by considering solutions which are functions of energy only. As soon as we would introduce a field term, or consider spatially inhomogeneous problems, we would have to resort to some form of particle-based discretization, and the solution of implicit equations would become a major issue. With an eye to the future particle-based solution of inhomogeneous problems, the easiest way out of this dilemma is to actually solve for the asymptotic expansion of f given by (4.5). That is, to write $f = f_0 + \lambda f_1$ and to solve the system

$$\text{(a)} \quad \partial_t f_0 = Q_0[f_0], \qquad \text{(b)} \quad \partial_t f_1 = Q_0[f_1] + Q_1[f_0]. \tag{4.8}$$

Now the time derivative of the zero order term f_0, which appears in (4.8)(b), can be replaced by (4.8)(a), and we actually solve

$$\begin{aligned} &\text{(a)} \quad \partial_t f_0 = Q_0[f_0], \\ &\text{(b)} \quad \partial_t f_1 = Q_0[f_1] + \int dp[S_1(p,p')Q_0[f_0](p',t) - S_1(p',p)Q_0[f_0](p,t)]. \end{aligned} \tag{4.9}$$

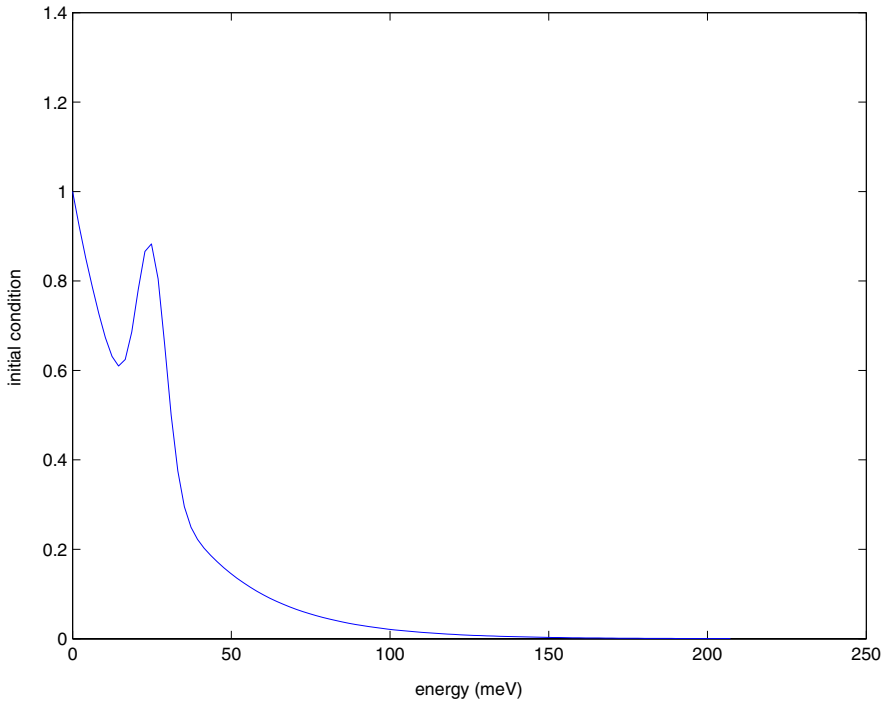

FIG. 4. *Initial condition for the Levinson equation.*

Equation (4.9)(a) is just the Boltzmann equation with the Fermi golden rule operator, and (4.9)(b) is also the same Boltzmann equation with an additional source term, which could be discretized using weighted particles. It is in this form that the numerical experiments below have been carried out, using the discretizations (4.2) and (4.4) for the operators Q_1 and Q_2.

We choose as initial condition (shown in Figure 4) the equilibrium Maxwellian with a second peak added. Thus we expect the second peak to be eliminated by the evolution of the Levinson equation as time advances. Figure 5 shows the solution f_λ of the Levinson equation (1.2) as a function of energy and time, and it exhibits the expected oscillations in time, albeit not to the same extent as the test example. To compare this solution with the asymptotic solution of (4.9), we smooth it in the same way as in the test example, i.e., by convoluting it with a Gaussian in time, shown in Figure 6. Figure 7 shows the solution of (4.9) for the same parameters. Figure 8 compares the full solution f_λ of the Levinson equation to the solution f_0 of the Fermi golden rule and $f_0 + \lambda f_1$ of (4.9) at different points in time. We observe that the solution f_0 of the Fermi golden rule has essentially reached steady state, while the full solution f_λ still evolves, i.e., the quantum effect causes a significantly longer relaxation time. This behavior is captured more or less by the asymptotic solution $f_0 + \lambda f_1$.

The structure of the equilibrium solution for the Fermi golden rule is determined by the fact that we have chosen a simple constant value of the lattice state frequency F in (4.6), corresponding to a δ-function collision potential [10]. This implies that the kernel of the Fermi golden rule operator Q_0 contains not only Maxwellians, but Maxwellians multiplied by arbitrary $\hbar\omega$-periodic functions of energy [7], [8], [12]. The steps in the equilibrium solution in the lower-right panel of Figure 8 represent the

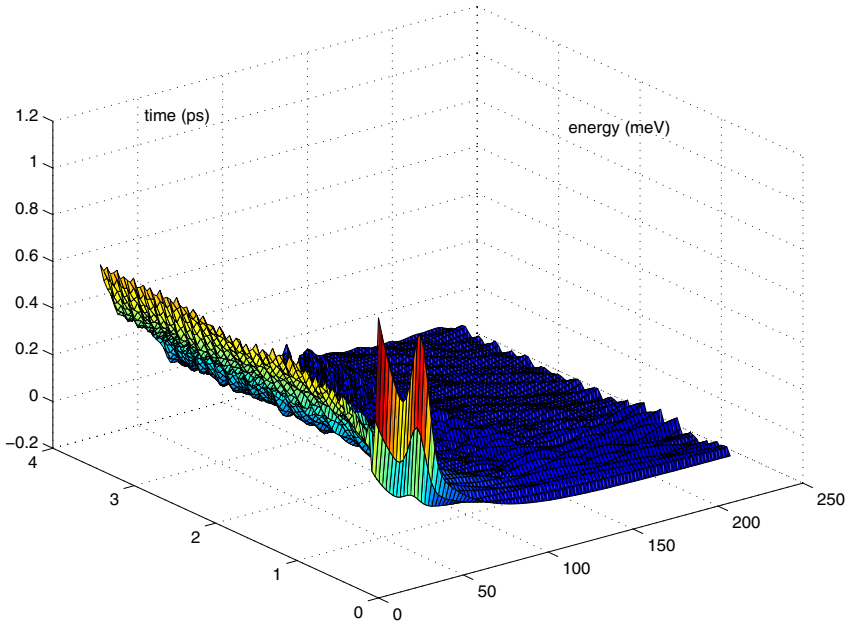

FIG. 5. *Solution of the Levinson equation.*

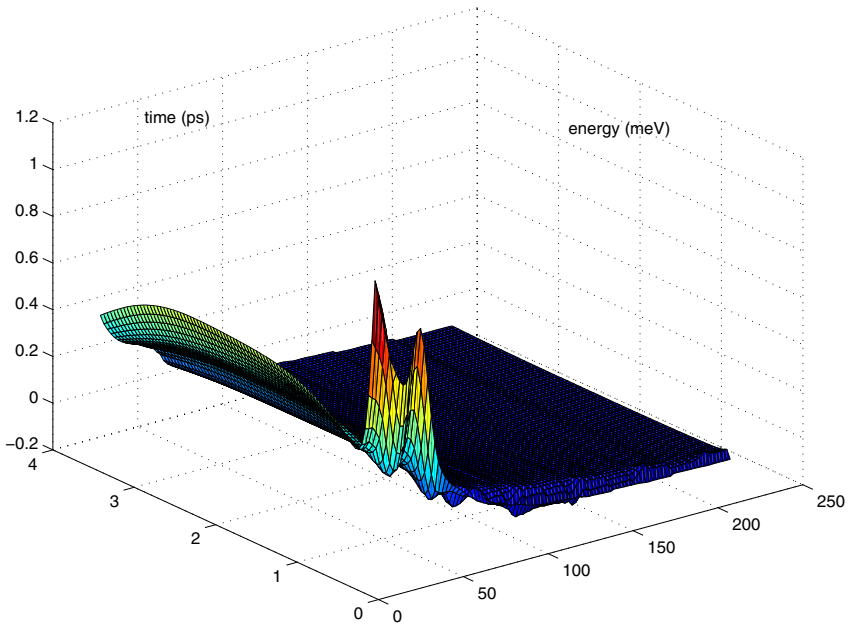

FIG. 6. *Filtered solution of the Levinson equation.*

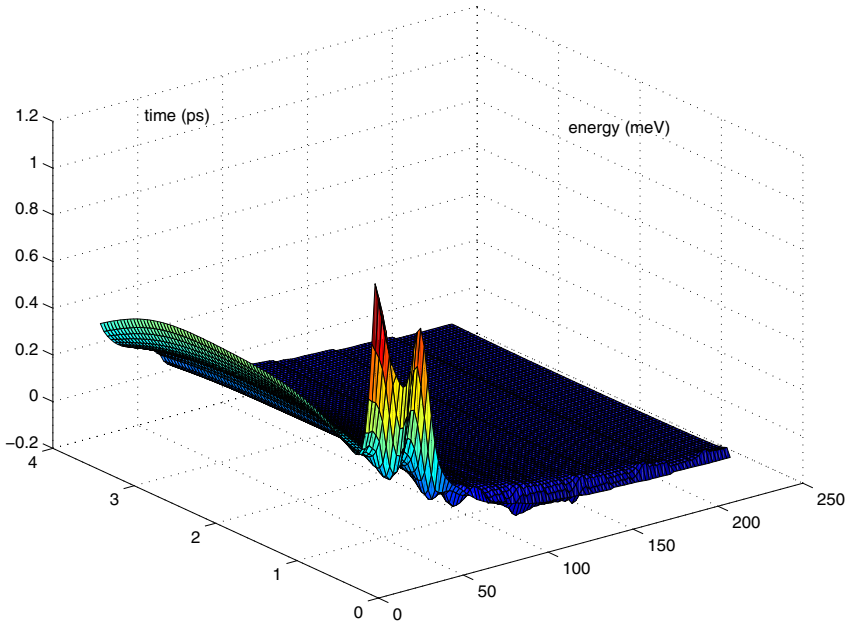

FIG. 7. *Approximate solution of the Levinson equation.*

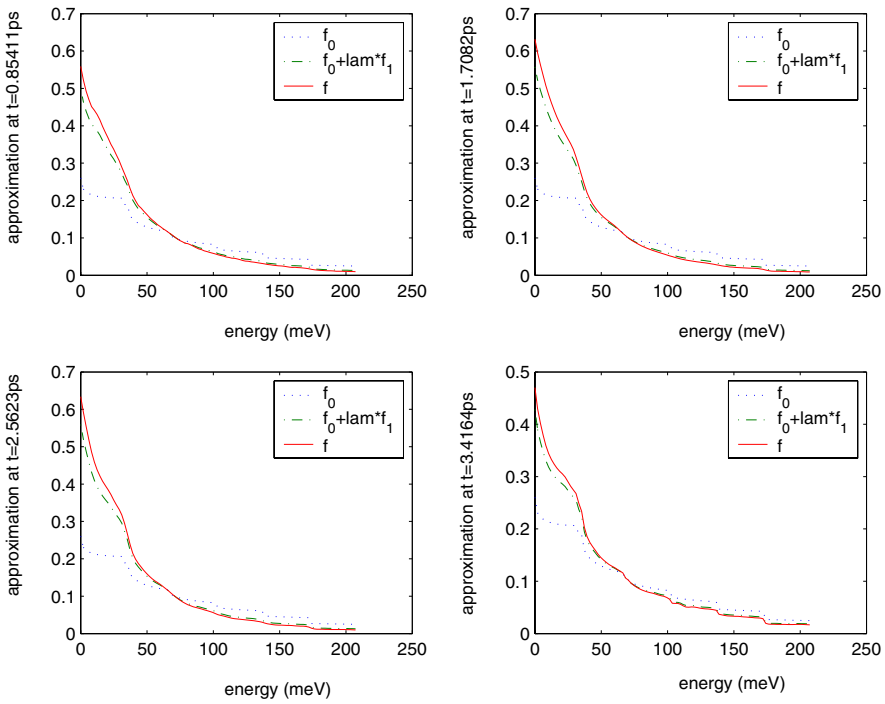

FIG. 8. *Snaphots of the solution and its approximations.*

projection of the initial solution into this space.

We were unable to continue the comparison beyond the given point in time due to memory constraints, since the solution of the Levinson equation requires time steps much smaller than λ to resolve the oscillations, and the storage of all previous time steps because of its nonlocality in time. It should be pointed out that the solution of the asymptotic system (4.9) does not suffer from these constraints, and (4.9) could be solved with much larger time steps on much longer timescales. The asymptotic solution $f_0 + \lambda f_1$ will eventually, however, converge to the same equilibrium solution, since the system (4.9) clearly has the same steady states as the original Fermi golden rule equation (1.2). Thus the quantum corrections give, at least in the absence of an electric field term, a purely transient effect.

5. Conclusions. Based on the Levinson equation, which in turn is derived from a weak interaction limit for the many body Schrödinger equation, we have derived a corrective term to the semiclassical Fermi golden rule collision operator. This corrective term is only mildly nonlocal in time in the sense that it is a local operator acting on the time derivative of the density function. It therefore renders itself much more easily to simulations on long timescales than did the original Levinson operator. We have shown the weak convergence of the corrected operator to the Levinson operator; i.e., we have proven the oscillatory limit for large times. Furthermore, we have demonstrated numerically the convergence of the solution to the Levinson equation towards the system resulting from the corresponding asymptotic expansion. From a numerical standpoint the complexity of this system is equivalent to that of solving a standard Boltzmann equation with additional source terms.

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