# Electron mobility in semiconductors. II.

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An extension is given to a previous calculation of the linear electric mobility of a single electron interacting only with lattice vibrations. These calculations are based on the path-integral representation of Feynman *et al.* for a polaron. They apply only in the macroscopic limit, the limit of small wave vectors in a representation of the electron's distribution function. The present calculation attempts to find the complete kernel of the path integral, which is no longer taken to be Markovian, to an accuracy of order $1/n$, where $n$ is the number of elapsed collisions. The kernel is found expressible in terms of functions of the time only. These functions satisfy soluble coupled integro-differential equations. We argue that the solution of these equations, which leads to the steady-state distribution function in Wigner electron coordinates $\vec{r}$ and $\vec{u}$ obtained previously, is the unique physical solution.

## I. INTRODUCTION

The desire to place electron transport in crystals on a first-principles basis has existed for a long time. The problem of interest in this paper is that of a single electron interacting only with the lattice vibrations of the crystal, which can be under the influence of a weak electric field $\vec{E}$. In other words, we have linear mobility and the effective-mass approximation in a nondegenerate semiconductor. Different approaches to calculating the polaron mobility have been taken. Feynman, Hellwarth, Iddings, and Platzman[1] eliminated the phonon coordinates from the problem, leading to an electron-density matrix in the form of a double path integral. Several calculations of mobility using the Feynman formula and a Boltzmann and/or variational technique[1-4] have been carried out in the past.

Just as the Feynman path-integral formulation of quantum mechanics can be reduced to the Schrödinger equation, so too can the double path integral for the density matrix be reduced to an integro-differential (ID) equation.[5] In a previous publication[6] (hereafter referred to as I), we attempted to solve this ID equation with a Markovian trial solution for the density matrix. The approach is based on classical Brownian motion,[7] where the random motion is assumed unaffected by the motion of the colloid particle. We assume in I that we can average out the memory effects of the previous motion of the electron. These memory effects are stored in the lattice in the complex amplitudes of vibration. Simplified models representing silicon and germanium gave encouraging results in regard to the values of the deformation-potential coupling constants, the temperature dependence of mobility, and the adherence to the Einstein diffusion relation. It turned out that for the typical semiconduction parameters considered there the electron-phonon interaction effectively occurs in a time interval only of the order of $10^{-2}$ of the periods of the most relevant lattice modes of vibration. Thus memory effects may be minimal, and the Markovian approach appears realistic.

In attempting to develop a means of calculating the non-Markovian corrections, we found that the previous results embodying an Einstein diffusion picture go beyond the Markovian approximation. Indeed, when slightly generalized, they represent the steady-state distribution function without approximation to within a factor of $(1/n)$, where $n$, the number of elapsed "collisions," is typically of the order of $10^8$ in room-temperature experiments.[8] This paper develops the reasons for this conclusion as we see them.

The key to obtaining a solution to the ID equation in I is the observation that in measuring electron diffusion and mobility we are averaging the distribution function in velocity and position over all velocities, and are concerned only with the macroscopic features of the remaining spatial distribution. This means that in a Fourier representation only very small wave-vector components (of the order of $1/\sqrt{n}$ times the Einstein diffusion length) are needed. It becomes possible to solve the ID equation using Taylor expansions in these small components, and up to second order in the wave vectors the Markovian trial solution becomes an exact solution of the ID equation. This raises a question, which is fundamental in many-body problems. Can we have a solution of the equation of motion which satisfies initial and boundary conditions, but does not necessarily represent the exact solution to the problem?

Let us develop these ideas mathematically, thereby gaining a perspective of the approach we shall take to the problem. As a first step in I we transformed the quantum-mechanical problem to the classical-like Wigner variables, electron space coordinate $\vec{r}$, velocity coordinate $\vec{u}$. In terms of these variables we defined a propagator (density matrix), which we called $\rho_W$ "closed," or $\rho_W(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;t)$, which we can think of as the probability of the electron's going from $\vec{r}_0,\vec{u}_0$, at time 0 to $\vec{r},\vec{u}$ at time $t$. In addition to a $\rho_W^{\text{closed}}$, we shall also need a $\rho_W$ "open", or $\rho_W(\vec{r}_N,\vec{u}_N,\ldots,\vec{r}_I,\vec{u}_I,\ldots,r_0,\vec{u}_0;\tau)$. We divide the time of propagation of the electron from 0 to $t$ into $N$ arbitrarily chosen intervals, $\tau_1,\tau_2,\ldots,\tau_I,\ldots,\tau_N$, separating times $t_1,t_2,\ldots,t_N$, with

$$\tau_I \equiv t_I - t_{I-1},\quad I=1,2,\ldots,N,\quad t_N\equiv t\ . \tag{1.1}$$

$\rho_W^{\text{open}}$ represents the electron's going from $\vec{r}_0,\vec{u}_0$ at time 0 to $\vec{r}_1,\vec{u}_1$ at time $t_1$, to $\vec{r}_2,\vec{u}_2$ at $t_2,\ldots$ to $\vec{r}_N,\vec{u}_N$ (or just plain $\vec{r},\vec{u}$) at time $t$; in other words, the probability of a path. $\rho_W^{\text{open}}$ is available explicitly. We shall show in Sec. III how it can be obtained from a double path integral given by Feynman *et al.* That integral describes the propagator of the electron after removal of lattice coordinates.

The relationship between $\rho_W^{\text{open}}$ and $\rho_W^{\text{closed}}$ is the following:

$$\rho_W(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;t)=\int_{-\infty}^{\infty}\rho_W(\vec{r}_N,\vec{u}_N,\ldots,\vec{r}_I,\vec{u}_I,\ldots,\vec{r}_0,\vec{u}_0;\tau)d^3r_{N-1}d^3u_{N-1}\cdots d^3r_1d^3u_1\ , \tag{1.2}$$

where performing the integrations on the right-hand side will be called "closing."

Physically, a Markovian process is one in which the time evolution of a particle depends only on the present, and not the past. Mathematically, a Markovian propagator must satisfy

$$\rho_W(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;t)=\int\rho_W(\vec{r},\vec{u};\vec{r}_I,\vec{u}_I;t-t_I)\rho_W(\vec{r}_I,\vec{u}_I;\vec{r}_0,\vec{u}_0;t_I)d^3r_Id^3u_I\ . \tag{1.3}$$

The propagator we use in I was modeled closely on a particle undergoing Brownian motion,[7] reducing, for $t\to\infty$, to

$$\rho_W^{\text{closed}}(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;t)\propto\exp[-(\vec{r}-\vec{r}_0)^2/(4a_0Dt)]\exp[-mu^2/(2k_BTb_0)]\ , \tag{1.4}$$

where $D$ is a diffusion constant. This is Einstein diffusion in space, along with the Maxwell velocity distribution, when parameters $a_0,b_0$, defined in Eq. (1.5), equal unity.

For finite $t$ the Markovian character of the full propagator becomes most easily apparent by examining its Fourier representation. In dimensionless variables[6] [time measured in units of $\beta^{-1}$, the "damping time," distances in terms of an "Einstein diffusion length," $(D/\beta)^{1/2}$], we have in I that

$$\rho_W(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;t)=(2\pi)^{-6}\int\int d^3k\,d^3w\times\exp[i\vec{k}\cdot(\vec{u}-\vec{u}_0e^{-t})]\times e^{i\vec{w}\cdot\vec{P}}\hat{\rho}(\vec{k},\vec{w},t)\ , \tag{1.5a}$$

$$\vec{P}\equiv\vec{r}+\vec{u}-\vec{r}_0-\vec{u}_0\ , \tag{1.5b}$$

$$\hat{\rho}(\vec{k},\vec{w},t)=e^F\ , \tag{1.5c}$$

$$F=-\tfrac{1}{2}(bk^2-2h\vec{k}\cdot\vec{w}+aw^2)\ , \tag{1.5d}$$

$$a=2a_0\int_0^t dt=2a_0t\ , \tag{1.5e}$$

$$b=2b_0\int_0^t e^{-2t}dt=b_0(1-e^{-2t})\ , \tag{1.5f}$$

$$h=-2h_0\int_0^t e^{-t}dt=-2h_0(1-e^{-t})\ , \tag{1.5g}$$

and we are here generalizing by also including a parameter $b_0$, which formerly was unity. The integral form of the coefficients in Eqs. (1.5e)—(1.5g) can be traced back to $\rho_W$ being the solution of a diffusion equation. When we Fourier represent $\rho_W(\vec{r},\vec{u};\vec{r}_I,\vec{u}_I;t-t_I)$ and $\rho_W(r_I,u_I;r_0,u_0;t_I)$, $t>t_I>0$ according to Eq. (1.5a) with wave vectors $\vec{k},\vec{w};\vec{k}\,',\vec{w}\,'$, respectively, and close by integrating over $\vec{P}_I$ and $\vec{u}_I$ we find integrals

$$\frac{1}{(2\pi)^3}\int\exp[i(\vec{k}e^{-(t-t_I)}-\vec{k}\,')\cdot\vec{u}_I]d^3u_I=\delta^3(\vec{k}e^{-(t-t_I)}-\vec{k}\,') \tag{1.6a}$$

and

$$\frac{1}{(2\pi)^3}\int\exp[i(\vec{w}-\vec{w}\,')\cdot\vec{P}_I]d^3P_I=\delta^3(\vec{w}-\vec{w}\,') \tag{1.6b}$$

that is, integrals representing Dirac $\delta$ functions. Further, we extend our definition (1.5f) in a convenient way by letting

$$b(t_I)\equiv 2b_0e^{-2t_I}\int_0^{t_I}e^{2t}dt\ . \tag{1.7}$$

We have

$$-\tfrac{1}{2}b(t-t_I)k^2-\tfrac{1}{2}b(t_I)k'^2=-\tfrac{1}{2}b(t)k^2$$

if $\vec{k}\,'=\vec{k}e^{-(t-t_I)}$.

We have, generally

$$F(\vec{k},\vec{w},t-t_I)+F(\vec{k}\,',\vec{w}\,',t_I)=F(\vec{k},\vec{w},t)\ . \tag{1.8}$$

It follows that $\rho_W$ is Markovian, Eq. (1.3).

We now see how to generalize to obtain $\rho_W$ "opened" at $N-1$ times. $\rho$ open will have a Fourier representation in terms of $2N$ wave vectors $\vec{k}_1,\ldots,\vec{k}_I,\ldots,\vec{k}_N$, $\vec{w}_1,\ldots,\vec{w}_I,\ldots,\vec{w}_N$, and again a Fourier transform

$$\hat{\rho}=e^F \tag{1.9a}$$

with $F$ a diagonal quadratic form

$$F=\sum_{I=1}^{N}F_I\ , \tag{1.9b}$$

$$F_I=-\tfrac{1}{2}(b_Ik_I^2-2h_Ik_Iw_I+a_Iw_I^2)\ , \tag{1.9c}$$

$$a_I = 2a_0(t_I - t_{I-1}) , \tag{1.9d}$$

$$b_I = b_0 e^{-2t_I} \int_{t_{I-1}}^{t_I} e^{2t} dt , \tag{1.9e}$$

$$h_I = -2h_0 e^{-t_I} \int_{t_{I-1}}^{t_I} e^{t} dt . \tag{1.9f}$$

We see that given the closed propagator $\rho_W(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0,t)$, and the information that it is Markovian, its open form is uniquely determined for us.

Let us now return to our ID equation of motion, which from I has the form

$$\frac{\partial \rho_W}{\partial t} + \vec{u}\cdot\vec{\nabla}_{\vec{r}}\rho_W = \lim_{\substack{N\to\infty,\\ \tau_I\to 0}} \sum_{I=1}^{N} \int V(\vec{r},\vec{u};\vec{r}_I,\vec{u}_I;t-t_I)\rho_W^{\text{open}} d^3r_{N-1} \cdots d^3u_1 , \tag{1.10}$$

where $V$ is some influence function (actually operator). Equation (1.10) has a unique Markovian solution. However, if $\rho_W$ is not assumed Markovian, then Eq. (1.10) does not fully determine $\rho_W$, not even $\rho_W^{\text{closed}}$. We can think of the closing procedure called for by Eq. (1.10) as a procedure of projection on a limited subspace. There exists, actually, a hierarchy of ID equations of motion, with the next equation relating $\rho$ open at one time to $\rho$ open at two times, etc. It is these equations that determine $\rho$ open fully. This situation is similar to the one encountered in the many-electron problem,[9] where one resorts to truncating, i.e., stopping the chain of equations at some point, and solving the last equation as best as one can with an approximation. Our response to the situation, to determine what is going on, is to solve the problem "open." In this paper we treat $\rho$ as a problem in $6N$ coordinates, where $N$ is a large number to be defined in terms of convergence of the double path integral specifying the density matrix of the electron.

Physically, our problem is manifestly not Markovian. The electron is influenced by the instantaneous deformation of the lattice, which deformation in turn, is determined by the previous path of the electron. The Markovian propagator of I, represented fully open in Eqs. (1.9), cannot be the exact solution of the problem, because it does not provide any links from the past to the present.

Still restricting ourselves to small wave vectors we shall learn that the ID equations of motion for $\rho$ open are generalized diffusion equations in wave-vector space, with exponential solutions. The most general Fourier representation of $\rho$ open will consequently be obtained by replacing the diagonal form for $F$ in Eq. (1.8) by a general quadratic form, with cross terms linking different time intervals. It is this form for $F$ that we use in subsequent sections.

It might be supposed that this form of solution will render the problem completely intractable. This is not so. For the steady-state closed propagator of interest here, we note that we shall only need certain sums of the coefficients appearing in the generalized quadratic form $F$. This is because upon closing one has

$$\vec{w}_I = \vec{w}_N, \quad \vec{k}_I e^{-(t-t_I)} = \vec{k}_N , \tag{1.11}$$

for $I=1,2,\ldots,N-1$. See Eqs. (1.6a) and (1.6b). This has the result that the wave vectors become common factors for large blocks of terms in $F$ allowing for direct summations of the coefficients in a block. These sums become the new unknowns. It will, accordingly, turn out that we can solve our problem by first assuming a great number of intervals $N$, and then finding equations for the desired sums of coefficients. These equations become ID equations as we let $N\to\infty$, with $t$ the only independent variable.

After obtaining equations of motion for $\rho$ open, which we do in Sec. II, we must show in Sec. III how to generalize the transformation to Wigner variables for our $6N$ coordinate problem. These details are needed to write down, in Sec. IV, a fully general form for the Fourier representation of $\rho$ open. Appendix A motivates our procedure of obtaining equations of motion for $\rho$ open by looking at the Feynman path-integral propagator for a single particle in a given potential. The mathematical details of reducing the ID equations of motion for $\rho$ open to equations for the coefficients in $F$ are relegated to Appendices B and C. In the last sections, V–VII, and in Appendix D, we show how to solve these latter equations, and obtain the desired coefficient sums for steady-state propagation. The outcome is a more complete physical solution for both $\rho$ open and $\rho$ closed than we obtained in I, with results for $\rho$ closed, the distribution function in the final $\vec{u}$ and $\vec{r}$, largely but not fully anticipated there.

## II. DERIVATION OF ID EQUATION

As mentioned, by eliminating lattice mode coordinates Feynman *et al.* obtained an expression for the propagator $\rho(\vec{R},\vec{R}';\vec{R}_0,\vec{R}'_0;t)$ taking the electron from $\vec{R}_0,\vec{R}'_0$ at time 0 to $\vec{R},\vec{R}'$ at time $t$ in the form of a double-path integral. We can write

$$\rho_N(\vec{R},\vec{R}';\vec{R}_0,\vec{R}'_0;t) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \rho(R_N,R'_N,\ldots,\vec{R}_I,\vec{R}'_I,\ldots,\vec{R}_0,\vec{R}'_0) d^3R_{N-1} \cdots d^3R'_1 ,$$
$$\vec{R} \equiv \vec{R}_N, \quad \vec{R}' \equiv \vec{R}'_N, \quad N > I > 0 . \tag{2.1}$$

We shall refer to the integrand on the right, the kernel of the double-path integral, as $\rho$ "open," and it shall be distinguished from the quantity on the left, $\rho$ "closed," by indicating its dependence on the multiplicity of variables involved.

Explicitly, $\rho$ open is[1,5,6]

$$\rho(\vec{R}_N,\vec{R}'_N,\ldots,\vec{R}_0,\vec{R}'_0;\tau)=\left[\prod_{I=1}^{N}\left[\frac{h\tau_I}{m}\right]^{-3}\right]\exp\left[\frac{im}{2\hbar}\sum_{I=1}^{N}\left[\frac{(\vec{R}_I-\vec{R}_{I-1})^2}{\tau_I}-\frac{(R'_I-R'_I)^2}{\tau_I}\right]-\frac{i}{\hbar}\sum_{I=1}^{N}\tau_I\sum_{I'=0}^{I-1}\tau_{I'+1}\Phi(\vec{R}_I,\vec{R}'_I;\vec{R}_{I'},\vec{R}'_{I'})\right], \tag{2.2a}$$

where

$$\Phi(\vec{R}_I,\vec{R}'_I;\vec{R}_{I'},\vec{R}'_{I'})=-\hbar\sum_K[S_{1K}(t_I-t_{I'})v_1(I,I')-S_{2K}(t_I-t_{I'})v_2(I,I')], \tag{2.2b}$$

$$(S_{1\vec{K}},S_{2\vec{K}})=\frac{2}{\hbar^2}|C_K|^2(\sin[w_{\vec{K}}(t_I-t_{I'})],\xi_{\vec{K}}/i\cos[w_{\vec{K}}(t_I-t_{I'})]), \tag{2.2c}$$

$$\left.\begin{matrix}v_1(I,I')\\ v_2(I,I')\end{matrix}\right\}=e^{i\vec{K}\cdot(\vec{R}_I-\vec{R}_{I'})}-e^{i\vec{K}\cdot(\vec{R}'_I-\vec{R}_{I'})}\pm e^{i\vec{K}\cdot(\vec{R}_I-\vec{R}'_{I'})}\mp e^{i\vec{K}\cdot(\vec{R}'_I-\vec{R}'_{I'})}, \tag{2.2d}$$

$$t_I=\sum_1^I\tau_{I'}, \tag{2.2e}$$

$$t\equiv t_N, \tag{2.2f}$$

$\xi_K=2n_K+1$, $n_K$=thermal number of phonons in longitudinal mode of vibration $\vec{K}$, of frequency $w_K$. $C_K$ is the electron-phonon coupling constant. We have changed the notation slightly from I to make the paper easier to read.

Equation (2.2a) differs from the usual expression in that we allow for differing time intervals $\tau_I$, $I=1,2,\ldots,N$. We suggest the reader refer to Appendix A, where we motivate our development with the example of a single particle in a potential. Throughout the paper we shall adopt the convention of showing $\rho$ depending on argument $\tau$, when we mean that it actually depends on the $N$ time intervals $\tau_I$. We take it that for $\rho_N$ closed defined in Eqs. (2.1) and (2.2) there will always exist for all physical arguments a limiting value, called $\rho(t)$ closed, in the following sense. Let $T$ be an upper limit on the total times of propagation of interest. Then there exists for any given positive number $\epsilon$, however small, some number $N$, such that given any number $N'>N$, and any choice of $N'$ positive time intervals $\tau'_I$,

$$|\rho_{N'}^{\text{closed}}(t)-\rho^{\text{closed}}(t)|<\epsilon$$

provided only

$$\tau'_I\le T/N \quad \text{for } I=1,2,\ldots,N'$$

and

$$t=\sum_1^{N'}\tau'_I\,.$$

With this assumption we can find $\rho$ closed for different times $t$, $0<t<T$, with the same number of intermediate variables, $R_1,\ldots,R_{N-1},R'_1,\ldots,R'_{N-1'}$, before going to the limit, $\epsilon\to0$ (see also Appendix A).

We can now easily generate ID equations of motion for $\rho$ open by formally partially differentiating with respect to the different $\tau_I$. Actually it will suffice for our work to differentiate only with respect to the last $\tau,\tau_N$, relying in due course on an implicit process of induction to solve our problem.

We have

$$\frac{\partial\rho(\vec{R}_N,\vec{R}'_N,\ldots,\vec{R}_0,\vec{R}'_0;\tau)}{\partial\tau_N}=\left[\frac{-3}{\tau_N}-\frac{im}{2\hbar\tau_N^2}[(\vec{R}_N-\vec{R}_{N-1})^2+(\vec{R}'_N-\vec{R}'_{N-1})^2]\frac{-i}{\hbar}\sum_{J=1}^{N}\tau_J\Phi(\vec{R}_N,\vec{R}'_N;\vec{R}_J,\vec{R}'_J)\right]\rho(\vec{R}_N,\vec{R}'_N,\ldots,\vec{R}_0,\vec{R}'_0;\tau),$$

and to lowest order in $\tau_N$,

$$\left[\frac{\partial}{\partial\tau_N}+\frac{\hbar}{2im}(\nabla^2_{R_N}-\nabla^2_{R'_N})\right]\rho^{\text{open}}=\frac{1}{i\hbar}\sum_{J=1}^{N}\tau_J\Phi(R_N,R'_N;R_J,R'_J)\rho^{\text{open}}, \tag{2.3}$$

as one can see by explicitly taking the Laplacian involved, omitting terms in which they operate on $\Phi$.

## III. TRANSFORMATION TO WIGNER FORMS AND FOURIER REPRESENTATIONS

To carry out the transformation to Wigner form[10] we first define variables

$$\vec{r}_I=(\vec{R}_I+\vec{R}'_I)/2 , \quad (3.1a)$$

$$\vec{y}_I=\vec{R}_I-\vec{R}'_I , \quad (3.1b)$$

where $I=0,1,\ldots,N$ and for $\rho$ closed we have the transformation

$$\rho_W(\vec{r}_N,\vec{u}_N;\vec{r}_0,u_0;t)=(m/h)^3\int\int \exp -i(m/\hbar)(\vec{y}_N\cdot\vec{u}_N-\vec{y}_0\cdot\vec{u}_0) \times\rho(\vec{r}_N+\vec{y}_N/2,\vec{r}_N-\vec{y}_N/2;\vec{r}_0+\vec{y}_0/2,\vec{r}_0-\vec{y}_0/2;t)d^3y_N\,d^3y_0 . \quad (3.2)$$

To deal with the transformation at intermediate times $s,t>s>0$, we need here to generalize from I, where the propagators were Markovian. In I, leaving out $\vec{r}$ variables we could write

$$\begin{aligned}\rho(y,y_0)&=\int_{-\infty}^{\infty}\rho(\vec{y},\vec{y}_s)\rho(\vec{y}_s,\vec{y}_0)d^3y_s\\ &=\int_{-\infty}^{\infty}\rho(\vec{y},\vec{y}'_s)\rho(\vec{y}_s,\vec{y})\delta^3(\vec{y}'_s-\vec{y}_s)d^3y_s d^3y'_s\\ &=\int_{-\infty}^{\infty}\rho(\vec{y},\vec{y}'_s)\rho(\vec{y}_s,\vec{y}_0)\\ &\quad\times\exp[i(m/\hbar)(\vec{y}'_s-\vec{y}_s)\cdot\vec{u}_s]d^3u_s d^3y'_s\,d^3y_s\\ &=\int_{-\infty}^{\infty}\rho(\vec{y},\vec{u}_s)\rho(\vec{u}_s,\vec{y}_0)d^3u_s .\end{aligned}$$

Here we notice from Eqs. (2.1) that $\Phi$, and indeed, $\rho$ open depend always on differences such as $\vec{R}_I-\vec{R}_{I-1}$ or $\vec{R}_I-\vec{R}'_1$, etc. If we associate variables $y$ with all leading coordinates (in their position on paper, or what comes to the same, in time), and variables $y'$ with all trailing coordinates, so that, for example,

$$\vec{R}_I-\vec{R}'_{I'}=\vec{r}_i-\vec{r}'_{I'}+(\vec{y}_I+\vec{y}'_{I'})/2 , \quad (3.3)$$

then we can generate $\rho(\vec{r}_N,\ldots,\vec{r}_0;\vec{y}_N,\ldots,\vec{y}_0,\vec{y}'_{N-1},\ldots,\vec{y}'_1;\tau)$ or $\Phi$ of these new arguments without ambiguity.

The Wigner transformation, for example, for $\rho$ open becomes:

$$\rho_W(\vec{r}_N,\ldots,\vec{r}_0;\vec{u}_N,\ldots,\vec{u}_0;\tau)\equiv\left[\frac{m}{h}\right]^{3N}\int_{-\infty}^{\infty}\exp[i(m/\hbar)(\vec{y}_N\cdot\vec{u}_N-\vec{y}_0\cdot\vec{u}_0)]\exp\left[i(m/\hbar)\sum_{I=1}^{N-1}\vec{u}_I\cdot(\vec{y}'_I-\vec{y}_I)\right] \times\rho(\vec{r}_N,\ldots,\vec{r}_0;\vec{y}_N,\ldots,\vec{y}_0;\vec{y}'_{N-1},\ldots,\vec{y}'_1;\tau) \times d^3y_N,\ldots,d^3y_0d^3y'_{N-1},\ldots,d^3y'_1 . \quad (3.4)$$

We notice that with this definition we again obtain $\rho_W$ closed if we integrate over intermediate variables $\vec{r}_{N-1},\ldots,\vec{r}_1,\vec{u}_{N-1},\ldots,\vec{u}_1$. Our analysis is built on the concept of jumps or random displacements in space and velocity. Rather than using $2N+2$ vector variables $\vec{r}_0,\ldots,\vec{r}_N,\vec{u}_0,\ldots,\vec{u}_N$, we shall use $2N$-vector variables

$$\delta\vec{P}_I=\vec{r}_I+\vec{u}_I-\vec{r}_{I-1}-\vec{u}_{I-1},\quad I=1,2,\ldots,N \quad (3.5a)$$

$$\delta\vec{u}_I=\vec{u}_I-\vec{u}_{I-1}e^{-\tau_I} , \quad (3.5b)$$

and end points $\vec{r}_0,\vec{u}_0,\vec{r}_N,\vec{u}_N$, thereby temporarily increasing the degrees of freedom. We are generalizing from I in using variables $\vec{P}_I=\vec{r}_I+\vec{u}_I$ and $\vec{u}_Ie^{-\tau_{I+1}}$ rather than $\vec{r}_I$ and $\vec{u}_I$. We are from now on again using dimensionless quantities throughout as in I, and Sec. I, here. Time is measured in units of $\beta^{-1}$, and distances in terms of the "Einstein diffusion length," $\sqrt{D/\beta}$. We shall have occasion to use the inverse of Eq. (3.5b), that is, expressions for each $\vec{u}_I$ in terms of the $\delta\vec{u}_I$. Actually, two expressions can be written down, depending on whether we solve "upwards from $I$," keeping $\vec{u}_N$, or "downwards," keeping $\vec{u}_0$. Simple algebra gives

$$\vec{u}_I^{+}\exp\left[-\sum_{I-1}^{N}\tau_{I'}\right]=\vec{u}_N-\sum_{I+1}^{N}\left[\delta\vec{u}_{I'}\exp\left[-\sum_{I'-1}^{N}\tau_{I''}\right]\right] , \quad (3.6a)$$

$$\vec{u}_I^{-}=\sum_{1}^{I}\left[\delta\vec{u}_{I'}\exp\left[-\sum_{I'+1}^{I}\tau_{I''}\right]\right]+\vec{u}_0\exp\left[-\sum_{1}^{I}\tau_{I'}\right] \quad (3.6b)$$

and, we have

$$\delta\vec{u}_i=\vec{u}_I^{-}-\vec{u}_{I-1}^{+}e^{-\tau_I} . \quad (3.6c)$$

We can take Eqs. (3.6) and (3.6b) as definitions of $\vec{u}_I^{+}$ and $\vec{u}_I^{-}$. Viewed as functions of the $(N+2)$ vectors $\vec{u}_0,\vec{u}_N,\delta\vec{u}_1,\ldots,\delta\vec{u}_N$, $\vec{u}_I^{+}$ and $\vec{u}_I^{-}$ are not equivalent. But when the condition

$$\sum_{I=1}^{N} \delta\vec{u}_I \exp\left[-\sum_{I+1}^{N}\tau_{I'}\right]=\vec{u}_N-\vec{u}_0 e^{-t} \qquad (3.6d)$$

which follows from the defining Eqs. (3.5a) and (3.5b) is imposed, $\vec{u}_I^{\,+}$ becomes equal, of course, to $\vec{u}_I^{\,-}$. In our $[6\times(N+2)]$-dimensional space, Eq. (3.4) becomes replaced by

$$\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\vec{P}_0,\vec{u}_0;\delta\vec{P},\delta\vec{u};\tau)$$
$$=\delta\left[\sum \delta\vec{P}_I-\vec{P}_N+\vec{P}_0\right]\delta\left[\delta u_I \exp-\sum_{I+1}^{N}\tau_{I'}-\vec{u}_N+\vec{u}_0 e^{-t}\right]$$
$$\times\left[\frac{m}{h}\right]^{3N}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp[i(m/\hbar)(\vec{y}_N\cdot\vec{u}_N-\vec{y}_0\cdot\vec{u}_0)]\exp\left[i(m/\hbar)\sum_{1}^{N-1}(\vec{u}_I^{\,+}\cdot\vec{y}\,'_I-\vec{u}_I^{\,-}\cdot\vec{y}_I)\right]$$
$$\times\rho(\vec{r}_N,\ldots,\vec{r}_1;\vec{y}_N,\ldots,\vec{y}_1;\vec{y}\,'_{N-1},\ldots,\vec{y}\,'_1;\tau)d^3y_N\cdots d^3y_0 d^3y'_{N+1}\cdots d^3y'_1\ , \qquad (3.7)$$

where *after* integrating over the various $y$ coordinates we introduce $P$ coordinates in favor of $r$ coordinates into the left-hand side. In view of the δ-function factors in Eq. (3.7), the introduction of the variables $\vec{u}_I^{\,+}$ and $\vec{u}_I^{\,-}$ of Eqs. (3.6) to replace $\vec{u}_I$ in Eq. (3.4) has no effect on the values of $\rho_W$ open. It will, however, be useful. It is possible to also convert the right- and left-hand sides of our ID equation to the new set of $[2\times(N+2)]$-vector variables as we shall see. What is the relationship between this calculation and the one envisaged so far in terms of the $2\times(N+1)$-vector variables $\vec{P}_0,\vec{P}_1,\ldots,\vec{P}_N,\vec{u}_0,\vec{u}_1,\ldots,\vec{u}_N$?

When in the $[6\times(N+2)]$-dimensional space we choose a point which is not on the surface described by the equations

$$\sum_{I+1}^{N}\delta\vec{P}_I-\vec{P}_N+\vec{P}_0=0\ , \qquad (3.8a)$$

$$\sum_{I=1}^{N}\delta\vec{u}_I\exp\left[-\sum_{I+1}^{N}\tau_{I'}\right]-\vec{u}_N+\vec{u}_0 e^{-t}=0 \qquad (3.8b)$$

then $\rho_W$ open, and both sides of the ID equation vanish. If the coordinates we choose do lie on the surface, then we are solving the same problem as before. We note that when we close, integration over the $2(N-1)$ intermediate coordinates $\vec{P}_1,\ldots,\vec{P}_{N-1},\vec{u}_1,\ldots,\vec{u}_{N-1}$ will be replaced by integration over all $2N$ jumps, $\delta\vec{P}_1,\ldots,\delta\vec{P}_N,\delta\vec{u}_1,\ldots,\delta\vec{u}_N$ [see (Eqs. 4.3)], the δ functions in (3.7) imposing the necessary restrictions. Our calculation continues by representing the open density matrix in the following way:

$$\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\vec{P}_0,\vec{u}_0;\delta\vec{P},\delta\vec{u};\tau)=(2\pi)^{-6N-6}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left[-i\vec{p}\cdot\left[\sum_{1}^{N}\delta\vec{P}_I-\vec{P}_N-\vec{P}_0)\right]\right.$$
$$\times\exp\left\{-i\vec{q}\cdot\left[\sum\delta\vec{u}_I\exp\left[-\sum_{I+1}^{N}\tau_{I'}\right]-\vec{u}_N-\vec{u}_0 e^{-t}\right]\right\}$$
$$\times e^{i\vec{w}\cdot\delta\vec{P}}e^{i\vec{k}\cdot\delta\vec{u}}\hat{\rho}_W(\vec{w},\vec{k};\vec{p},\vec{q};\tau)d^3w\,d^3k\,d^3p\,d^3q\ , \qquad (3.9a)$$

with

$$e^{i\vec{w}\cdot\delta\vec{P}}\equiv\exp\left[i\sum_{1}^{N}\vec{w}_I\cdot\delta\vec{P}_I\right]e^{i\vec{k}\cdot\delta\vec{u}}\equiv\exp\left[-\sum_{1}^{N}\vec{k}_I\cdot\delta\vec{u}_I\right] \qquad (3.9b)$$

$$\hat{\rho}_W(\vec{w},\vec{k};\vec{p},\vec{q};\tau)\equiv\hat{\rho}_W(\vec{w}_N,\ldots,\vec{w}_1;\vec{k}_N,\ldots,\vec{k}_1;\vec{p},\vec{q};\tau)\ , \qquad (3.9c)$$

$$d^3w\,d^3k\equiv d^3w_N\cdots d^3w_1 d^3k_N\cdots d^3k_1\ , \qquad (3.9d)$$

$$\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\vec{P}_0,\vec{u}_0;\delta\vec{P},\delta\vec{u};\tau)\equiv\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\vec{P}_0,\vec{u}_0;\delta\vec{P}_N,\ldots,\delta\vec{P}_1;\delta\vec{u}_N,\ldots,\delta\vec{u}_1;\tau)\ . \qquad (3.9e)$$

$\rho_W$ open in Eq. (3.4) depends on the $(N+1)$ vectors $\vec{r}_0, \vec{r}_1, \ldots, \vec{r}_N$. However, we can always take the origin at $\vec{r}_0$ (or in $P$ space at $\vec{P}_0$), i.e., subtract $\vec{r}_0$ from every variable. It follows that with $N$-independent vectors $w_I$ in Eq. (3.9a) we have full generality. We, therefore, may take $\hat{\rho}_W(\vec{w},\vec{k};\vec{p},\vec{q};\tau)$ independent of $\vec{p}$, thereby reproducing the δ-function behavior on $P$ in Eq. (3.7). The situation with the $u$ variables is somewhat different. It would be unphysical to choose an origin at $\vec{u}_0$. However, suppose we bring in a dependence on one more wave vector, for example, $\vec{q}_0$, by adding the factor $\exp(i\vec{q}_0\cdot\vec{u}_0 e^{-t})$. In that case, since we now have $(N+2)$ wave vectors, we can again take $\rho_W(\vec{w},\vec{k};\vec{p},\vec{q},q_0;\tau)$ independent of $\vec{q}$ without loss of generality, yielding the second δ function in Eq. (3.7). Now in our treatment we are making the physical assumption that in the steady state the initial velocity $\vec{u}_0$ has, indeed, thermalized; that is, $\vec{q}_0$ will not come out anomalously large. Our whole development bears out that this happens, so that $\exp(i\vec{q}_0\cdot\vec{u}_0 e^{-t})$ may be set equal to unity, and the degree of freedom dropped. We summarize

$$\vec{P}_0 \to 0,\quad \vec{u}_0 \to 0,\quad \hat{\rho}_W(\vec{w},\vec{k};\vec{p},\vec{q};\tau) \to \hat{\rho}_W(\vec{w},\vec{k};\tau)\ . \tag{3.9f}$$

The point about splitting $\delta u_I$ into $u^+$ and $u^-$, Eq. (3.6c), is that this procedure removes ambiguity when transforming the right-hand side of the equation of motion, Eq. (2.3), to Wigner variables. See Appendix B, where the transformation is carried out, and we make the Taylor expansion in wave vectors.

## IV. TRIAL SOLUTION

It will turn out to be convenient to make a time-dependent change of scale in the $k$-wave vectors. We let

$$\tilde{\vec{k}}_I \equiv \vec{k}_I \exp\left[\sum_{I+1}^{N} \tau_{I'}\right], \tag{4.1a}$$

$$\delta\tilde{\vec{u}}_I \equiv \delta\vec{u}_I \exp\left[-\sum_{I+1}^{N} \tau_{I'}\right], \tag{4.1b}$$

and

$$e^{i\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}}} \equiv e^{i\vec{k}\cdot\delta\vec{u}}\ , \tag{4.1c}$$

[see (Eq. 3.9b)]. In terms of these variables, the Fourier representation of our trial solution is following the notation of Eqs. (3.9):

$$\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\tilde{\vec{u}};\tau) = (2\pi)^{-(6N+6)} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left[-i\vec{p}\cdot\left[\sum_{1}^{N} \delta\vec{P}_I - \vec{P}_N\right]\right] \exp\left[-i\vec{q}\cdot\left[\sum \delta\tilde{\vec{u}}_I - \vec{u}_N\right]\right]$$
$$\times e^{i\vec{w}\cdot\delta\vec{P}} e^{i\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}}} \hat{\rho}(\vec{w},\tilde{\vec{k}};\tau) d^3w\, d^3\tilde{k}\, d^3p\, d^3q\ , \tag{4.2a}$$

$$\hat{\rho}(\vec{w},\tilde{\vec{k}};\tau) = \exp-\left[\tfrac{1}{2}F(\vec{w},\tilde{\vec{k}};\tau)\right]\ , \tag{4.2b}$$

$$F(\vec{w},\tilde{\vec{k}};\tau) = \sum_{I=1}^{N}\sum_{I'=1}^{I} \left[A_{II'}(\tau)\vec{w}_I\cdot\vec{w}_{I'} - H_{II'}(\tau)(\tilde{\vec{k}}_I\cdot\vec{w}_{I'} + \vec{w}_I\cdot\tilde{\vec{k}}_{I'}) + B_{II'}(\tau)\tilde{\vec{k}}_I\cdot\tilde{\vec{k}}_{I'}\right]\ . \tag{4.2c}$$

Here $A_{II'}$, $H_{II'}$, and $B_{II'}$ are coefficients which are to be determined from the ID equation of motion. On physical grounds we expect that $A_{II'}$ will be a function of $\tau_I, \tau_{I-1}, \ldots, \tau_{I'+1}$, but of none of the other $\tau$'s. [One can actually see this by comparison with the exact form Eq. (2.2a).] Because of the implied time dependence of $\delta\tilde{\vec{u}}_{I'}$, $H_{II'}$ and $B_{II'}$ may also depend on $\tau_N, \ldots, \tau_{I+1}$. To ensure time inversion symmetry $\vec{k}_I\cdot\vec{w}_{I'}$ and $\vec{w}_I\cdot\vec{k}_{I'}$ are taken to have the same coefficient. As we shall see, all the unknown coefficients can be found from the ID equations (differentation with respect to every $\tau_I$ produces a new ID equation). We shall only need certain partial sums of these coefficients. Let us close Eq. (4.2a) [see Eq. (1.1)]. We find

$$\rho_W(\vec{P}_N,\vec{u}_N;\tau) \equiv \int \rho_W(\vec{P}_N,\ldots,\vec{P}_1,\vec{u}_N,\ldots,\vec{u}_1;\tau) d^3P_{N-1}\cdots d^3P_1 d^3u_{N-1}\cdots d^3u_1$$
$$= \int \bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\tilde{\vec{u}};\tau) d^3\delta P_N \cdots d^3\delta P_1 d^3\delta\tilde{u}_N \cdots d^3\delta\tilde{u}_1 \tag{4.3a}$$
$$= (2\pi)^{-6} \int e^{i\vec{p}\cdot\vec{P}_N} e^{i\vec{q}\cdot\vec{u}_N} \hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};\tau) d^3p\, d^3q\ , \tag{4.3b}$$

$$\hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};\tau) = \exp\left[-\tfrac{1}{2}\sum_{I=1}^{N}\sum_{I'=1}^{I}(p^2A_{II'} - 2\vec{p}\cdot\vec{q}H_{II'} + q^2B_{II'})\right]\ . \tag{4.3c}$$

To find the transport coefficients, mobility, and diffusion constant, we only need $\rho_W$ closed. We see that $\rho_W$ closed requires a very limited subcollection of the Fourier transforms $\hat{\rho}(\vec{w},\vec{k};\vec{\tau})$.

We remember from I that the values required there of $w,k$ ($p$ and $q$ here) are of the order of $1/\sqrt{n}$, where $n$ is the number of elapsed collisions. The reasons for this were that we only needed the average of $\rho_W$ $(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;\tau)$

over all $\vec{u}$, and that in space the distribution was macroscopic. It follows that we can restrict out treatment, i.e., range of solutions, again to small wave vectors, and can again stop at a quadratic form for $F$. We shall see that our trial solution, Eqs. (4.2b) and (4.2c) is again a solution of the ID equation to order $1/n$, and it satisfies physical initial and boundary conditions. We notice that this time the solution is not Markovian, coefficients $A_{II}$, etc., $I \neq I'$, linking what happens at $t_I$ to what happens at $t_{I'}$. It is general in $6N$ degrees of freedom.

## V. COEFFICIENT SUMS

Upon closing we find (see Appendix B) that rather than requiring a knowledge of all the coefficients $A_{II'}$, $B_{II'}$, and $H_{II'}$, we only require certain sums of these in order to finally determine $\rho$ closed, that is, the distribution function in $\vec{u}$ and $\vec{r}$ at the final time $t$. These sums are the following:

$$A_1(J) \equiv A_1(\tau_1, \ldots, \tau_J) \equiv \sum_{I=1}^{J} \sum_{I'=1}^{I} A_{II'} , \tag{5.1a}$$

$$A_2(J) \equiv A_2(\tau_{J+1}, \ldots, \tau_N) \equiv \sum_{I=J+1}^{N} \sum_{I'=J+1}^{I} A_{II'} , \tag{5.1b}$$

$$A_3(J) \equiv A_3(\tau_1, \ldots, \tau_N) \equiv \sum_{I=J+1}^{N} \sum_{I'=1}^{J} A_{II'} , \tag{5.1c}$$

$$A \equiv A(\tau_1, \ldots, \tau_N) \equiv \sum_{I=1}^{N} \sum_{I'=1}^{I} A_{II'} , \tag{5.1d}$$

$$A = A_1 + A_2 + A_3 , \tag{5.1e}$$

Similar definitions apply for the sums $B, B_1, \ldots, H, H_1, \ldots$. Figure 1 illustrates the various regions in $I$-$I'$ space over which one is summing to get the variously subscripted functions.

We shall assume that

$$A(\tau_1, \tau_2, \ldots, \tau_N) = A(\tau_1 + \tau_2 + \cdots + \tau_N) = A(t) , \tag{5.2}$$

and similar dependencies for $B$ and $H$. We can justify this assumption in a number of ways. First, if our limiting procedure leads to a physical distribution function, $A$, $B$, and $H$ cannot depend on the individual $\tau$'s, which tend towards zero, but rather only on the total $t$. We see in Appendix A that a definition in terms of a similar limiting procedure for the propagator of a particle in a potential, $K$ closed, leads to the Schrödinger equation, and consequently $K$ closed, as we define it there, depends on $t$ only. Similarly, our definition for $\rho$ open will ultimately lead to its hierarchy of closed wave equations. Second, and more direct, in regard to $K$ closed we can always, given its definition in Appendix A, construct a proof by induction to validate its dependence on the overall $t$ only. In the case of the coefficients here such a proof by induction would assume a known solution for $A(t' = \tau_1 + \cdots + \tau_{N-1})$, $B$, and $H$, to the coupled equations we shall obtain for these functions, and then the extension of these solutions to $t' + \tau_N$. Since, as we shall see, the functions involved are either linear in $t$ or simple exponentials of $t$, such a proof is straightforward. We take the more direct approach via Eq. (5.2) for simplicity.

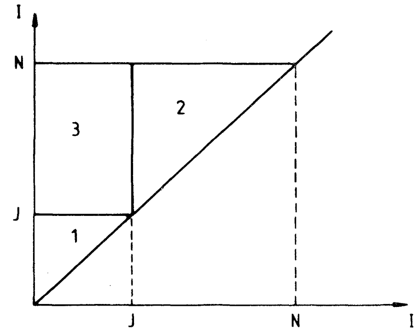


FIG. 1. Regions in $I$-$I'$ space which yield the partial sums $A_1, B_1, H_1, \hat{H}_1$; $A_2, B_2, H_2, \hat{H}_2$; and $A_3, B_3, H_3, \hat{H}_3$.

The coefficients $A$, $A_1$, $A_2$, $A_3$, etc., have certain functional relationships to each other, which it will be important to know. For later use, let us set

$$t_J \equiv s .$$

We shall ultimately think of $s$ as a continuous variable, $t > s > 0$. Because the coefficients $A_{II'}$ are functions of only the intervening time intervals $\tau_1, \ldots, \tau_{I'+1}$ but not of $I$ itself, we see that in accordance with Eq. (5.2)

$$A_1(\tau_1, \ldots, \tau_J) \equiv A_1(s) = A(s) . \tag{5.3a}$$

On the other hand, because of the time-dependent scale factors associated with $\vec{\delta u}_I$, and $\vec{k}_I$, $1 \le I \le N$, we must have

$$H_1(J) e^{(t - t_J)} \equiv H_1(t,s) e^{(t-s)} = H(s) \tag{5.3b}$$

and

$$B_1(J) e^{2(t - t_J)} \equiv B_1(t,s) e^{2(t-s)} = B(s) . \tag{5.3c}$$

Similarly one has

$$A_2(J) \equiv A_2(t,s) = A(t-s) , \tag{5.4a}$$

$$B_2(J) \equiv B_2(t,s) = B(t-s) , \tag{5.4b}$$

$$H_2(J) \equiv H_2(t,s) = H(t-s) . \tag{5.4c}$$

It is the individual coefficients in $A_3, B_3, H_3$ that couple the past, i.e., $t_I < s$ to the present, i.e., $t > t_I > s$. We now notice that because of their definitions in Eq. (5.1e), $A_3, B_3, H_3$ are also functionally determined by $A(t), B(t), H(t)$. From Eqs. (5.3a) and (5.4a),

$$A_3(t,s) = A(t) - A(s) - A(t-s) , \tag{5.5a}$$

$$B_3(t,s) = B(t) - e^{-2(t-s)} B(s) - B(t-s) , \tag{5.5b}$$

$$H_3(t,s) = H(t) - e^{-(t-s)} H(s) - H(t-s) . \tag{5.5c}$$

## VI. SOLUTIONS FOR COEFFICIENTS WHEN $A_3 = B_3 = H_3 = 0$

The calculation of the right- and left-hand sides of the ID equation of motion Eq. (2.2), are outlined in Appendices B and C. When we equate the respective coefficients of $q^2$, $\vec{p} \cdot \vec{q}$, and $p^2$ found on each side, we get the following three coupled ID equations for functions $A(t)$, $B(t)$, and $H(t)$:

$$\frac{-\beta}{2}\dot{B}(t)=\int_0^t ds\sum_{\vec{K}}[G_{1\vec{K}}(t-s)e^{-(t-s)}-G_{2\vec{K}}(t-s)n(t,s)]\ ,\tag{6.1a}$$

$$\beta[B(t)+\dot{H}(t)]=\int_0^t ds\sum_{\vec{K}}\{G_{1\vec{K}}(t-s)(1+e^{-(t-s)})-G_{2\vec{K}}(t-s)[n(t,s)-m(t-s)]\}\ ,\tag{6.1b}$$

$$-\beta[\dot{A}(t)/2+H(t)]=\int_0^t ds\sum_{\vec{K}}[G_{1\vec{K}}(t-s)+G_{2\vec{K}}(t-s)m(t,s)]\ ,\tag{6.1c}$$

where

$$G_{1\vec{K}}=[S_{1\vec{K}}(t-s)\sin\Lambda_K-S_{2K}(t-s)\cos\Lambda_K](2L^2K^2/3)\exp[-K^2R(t,s)]\ ,\tag{6.1d}$$

$$G_{2\vec{K}}=[S_{1K}(t-s)\cos\Lambda_K+S_{2K}(t-s)\sin\Lambda_K](2LK^2/3)\exp[-K^2R(t,s)]\ ,\tag{6.1e}$$

$$L=\hbar\beta/(2k_BT)\ ,\tag{6.1f}$$

$$\Lambda_K=LK^2(1-e^{-(t-s)})\ .\tag{6.1g}$$

Here we have changed sums over $t_J$ to integrals over $s\equiv t_J$. $T$ is temperature, $k_B$ is the Boltzmann constant, and $n,m,$ and $R$ are functions of $t$ and $s$ through

$$R(t,s)=A_2+2H_2+B_2+f(H_3+B_3)+f^2B_1\ ,\tag{6.2a}$$

$$2m(t,s)=2A_2+2H_2+2fH_1+A_3+H_3(1+f)\ ,\tag{6.2b}$$

$$2n(t,s)=2H_2+2B_2+2fB_1+H_3+B_3(1+f)\ ,\tag{6.2c}$$

with

$$f=1-e^{(t-s)}\ .\tag{6.2d}$$

To arrive at a solution of these equations, we start by setting $A_3=B_3=H_3=0$. Comparison with the earlier work (I) then shows that the resulting equations are equivalent to those implied there, but not written down, if we identify $A(t)$ here with $a(t)$ there, $B(t)$ with $b(t)$, and $H(t)$ with $h(t)$. In I we substituted trial solutions for these functions directly into the equation of motion, and fitted parameters. Here we have explicitly the equations which must be satisfied by our functions $A(t)$, etc., and shall solve them for steady-state conditions.

To discuss these equations we start by simplifying our notation, writing, for example, Eq. (6.1a) as

$$-(\beta/2)\dot{B}(t)=G_1(e^{-T})-G_2n\ ,\tag{6.3a}$$

$$T=t-s\ .\tag{6.3b}$$

Let us also eliminate the functions $A(s),B(s),H(s)$. Using Eqs. (5.5) we can write (with $A_3=B_3=H_3=0$)

$$A(s)=A(t)-A(t-s)\ ,\tag{6.4a}$$

$$B(s)=B(t)-B(t-s)\ ,\tag{6.4b}$$

$$H(s)=H(t)-H(t-s)\ .\tag{6.4c}$$

Substituting from Eqs. (6.2b) and (6.2c) we obtain

$$\frac{-\beta}{2}\dot{B}(t)+B(t)G_2(1-e^T)=G_1(e^{-T})-G_2(H_2+e^TB_2)\ .\tag{6.5}$$

Given our expressions for $G_{1K},G_{2K}$ and $S_{1K},S_{2K}$ in Eq. (2.1c), as well as the presence of the exponential factor in Eqs. (6.1d) and (6.1c), the analytic solutions of Eqs. (6.1a)—(6.1c) must be very complex. Such complexities have not been observed in the steady-state distribution function, and, physically we do not expect them to propagate. We are led to assume that they are associated with transients, especially as they are tied up with the abrupt beginning of the integrals at $s=0$. If we extend the integrals (time of propagation), back to $s=-\infty$, the complexities go away. Numerically this extension has no effect on the integrals in Eqs. (6.1). The reason lies with the oscillating nature of the functions $G_{1K},G_{2K},S_{1K},S_{2K}$ combined with the rapid decay of the factor $-\exp[K^2R(t,s)]$ in Eqs. (6.1d) and (6.1e). The latter, when determined in a fully self-consistent way from the solution of our equations, turns out to go typically as $\exp[-10^4(t-s)]$. In units of $\beta^{-1}$, we recall, $t$ is $\approx 10^8$, and $s$ is going negative from $t=0$.[13]

It is particularly important that we do not include transient effects in the functions $A(t)$, $B(t)$, $H(t)$, that do not belong in the coefficients $A_{JJ'}$, etc., themselves while describing steady-state propagation near the final time $t$. If we did include these effects we would have spurious contributions to the functions that are sums of these latter coefficients only, namely to $A(t-s)$, $B(t-s)$, $H(t-s)$, $(t-s)\leq 1/\beta$. It is at these final times that the main action of the influence function takes place in our ID equation.

With all this in mind we extend the propagation to formally start at $s=-\infty$ rather than at $s=0$ in our integrals on the right-hand side of Eqs. (6.1a)—(6.1c). With this procedure all expressions in Eq. (6.5) other than $B(t)$, $\dot{B}(t)$ become numbers, rather than functions. We show in Appendix D that this is true even though $R(t,s)$ is ostensibly a function of $t$ as well as $t-s$. We also give there forms equivalent to Eq. (6.5) for the two other original equations (6.1b) and (6.1c). We now have a coupled system of three differential equations with simple, physical solutions. Subject to the boundary condition $A(0)=B(0)=H(0)=0$, these solutions are given by

$$A(t)=2a_0t\ ,\tag{6.6a}$$

$$B(t)=b_0(1-e^{-2t})\ ,\tag{6.6b}$$

$$H(t)=-2h_0(1-e^{-t})\ ,\tag{6.6c}$$

with

$$h_0=(a_0+b_0)/2\ , \qquad (6.6d)$$

$$a_0=-\frac{G_1[\exp(-T)]}{G_2(1-e^{-T})}\ , \qquad (6.6e)$$

$$b_0=(1/\beta)[2a_0G_2(T)+G_1]\ , \qquad (6.6f)$$

subject to the condition

$$G_2(e^T-1)=\beta\ . \qquad (6.6g)$$

These results are closely similar to those obtained in I and gives physical results consistent with them. (Factors $2L^2$ and $2L$ have here been absorbed into our definitions of $G_1$ and $G_2$, respectively.) Equation (6.6g) fixes the value of $\beta$, and comes out as a subsidiary condition explicitly because of our choice of time units, i.e., choosing a simple exponential, e.g., $e^{-t}$ in $H(t)$. Checking we find that for Eqs. (6.6a)—(6.6c) the additive properties obtained by combining Eqs. (5.3) and (6.4) are also satisfied. For example, for B,

$$B(t)-e^{-2(t-s)}B(s)-B(t-s)=0\ . \qquad (6.7)$$

Thus Eqs. (6.6) not only satisfy Eq. (6.5) and its two complementary Eqs. (D1a) and (D1b), but the original Eqs. (6.1) with $A_3$, $B_3$, $H_3$ set equal to zero.

We recall that Eq. (6.6e), which also appears in I, typically gives values of $a_0$ very close to unity, thereby guaranteeing the Einstein relation [see Eq. (1.4)]. Actually,

$$G_1\approx G_1(e^{-T})\approx -G_2(1-e^{-T})\approx -G_2(T)\approx -G_2(e^T-1)=-\beta$$

so that from (6.6f), also $b_0\approx 1$, giving a near Maxwell tail to the velocity distribution, see Eq. (1.3). Thus, the theory shows independently of any assumption the exact behavior of the high-velocity end of the distribution function, a feature of which we were not aware when writing I. With $b_0\approx 1$, $b_0$ was set $=1$ in I, we will get the same encouraging physical results as before for temperature dependence, adherence to the Einstein relation, and deformation-potential coupling constants for semiconductor models of silicon and germanium.

## VII. GENERAL SOLUTION

Even if at the outset we retain $A_3$, $B_3$, $H_3$, Eqs. (6.8) provide a steady steady-state solution. We are to think of $A_3$, $B_3$, and $H_3$ as given by Eqs. (5.5), that is, defined by the functions $A$, $B$, and $H$, and as being substituted in this form into the general equations, (6.1). Now for the solutions given in Eqs. (6.6), as noted, $A$, $B$, and $H$ each satisfy an additive property, such as Eq. (6.7) for $B$. In other words, Eqs. (6.6) lead to the vanishing of $A_3$, $B_3$, $H_3$ as given in Eqs. (5.5). It follows that $A(t)$, $B(t)$, and $H(t)$ as given by Eqs. (6.6) are also steady-state solutions of the original ID Eqs. (6.1).

The factor $\exp[-K^2R(t,s)]$ aside, Eqs. (6.1a)—(6.1c) are a set of linear inhomogeneous equations. We know, in particular, from the work of Volterra[11] that linear inhomogeneous integral equations have unique solutions. (Volterra identified linear integral equations with equivalent sets of algebraic equations by dividing the range of the independent variable into discrete intervals. If the range is divided into $n$ intervals, one integral equation becomes a set of $n$ linear inhomogeneous algebraic equations with $n$ unknowns.)

For the solution in Eqs. (6), $R(t,s)$ becomes set exactly at

$$R(t,s)=a_0[\exp(-T)-1+T],\quad T\equiv t-s\ . \qquad (7.1)$$

We now note the qualitative (and quantitative) physical success obtained earlier with our solution, for $\rho_W$ closed. We also note that no iteration procedure about our solution is possible, since it, itself, is an exact solution. Thus, we do not expect that there will be another physically acceptable steady-state solution to Eqs. (6.1). Such an additional solution would have to result from an overall self-consistent alternative to the characteristic exponentially decaying behavior of $\exp[-K^2R(t,s)]$. These considerations lead us to suppose that in Eqs. (6.6) we are proposing the unique physical solution to Eqs. (6.1).

Let us review the situation. The picture of an electron as an erratic particle absorbing or emitting a single phonon at a time is not under observation, and does not play a part in our analysis. We see our quantum-mechanical equations of motion as compatible with the picture observed in transport experiments of an electron as a steadily propagating macroscopic distribution. These equations depict the distributed electron as continuously experiencing simultaneous recoil from interaction with a quasicontinuous spectrum of modes of vibration. Continuous diffusion under the influence of a steady thermodynamic force becomes a plausible description.

To solve the macroscopic steady-state problem of interest to us we can restrict ourselves to small wave vectors. For small wave vectors $k_{I'},w_{I'}$ we can, as we have seen, make a Taylor expansion of the right side of the equation of motion, which consists of the influence function acting on $\rho$ open. By differentiating $\rho$ open with respect to each of the $\tau_I$'s, $N\geq I\geq 1$, in turn we obtain $N$ generalized diffusion equations for $\rho$ of the form

$$\frac{\partial\hat{\rho}^{\rm open}}{\partial\tau_I}=Q(k_{I'},w_{I'})\rho^{\rm open},\quad N\geq I\geq 1,\quad N\geq I'\geq 1 \qquad (7.2)$$

where $Q(k_{I'},w_{I'})$ is a quadratic form in $k_{I'},w_{I'}$. The only possible self-consistent solution to these equations is a generalized Gaussian, such as the one that is given in Eq. (4.2c). Since a solution of these equations does exist, it is after all given in Eq. (2.2), and, since, we have written down the most general possible Gaussian, we must presume that the $[3N\times(N+1)/2]$ coefficients $A_{II'}$, $B_{II'}$, $H_{II'}$ suffice to accommodate the solution of Eq. (7.2). A proof showing that we have just the appropriate number of coefficients is outlined in Appendix E. The solution of Eq. (7.2) constitutes the desired form for $\rho$ open.

We can find the subset of transform coefficients $\hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q},t)$ which we need to find the distribution function, i.e., $\rho$ closed, by solving directly for certain overall sums, rather than finding all the individual coefficients $A_{II'}$, etc., themselves. The final distribution function in $\vec{r}$ and $\vec{u}$ agrees with the Markovian result obtained earlier in I, with certain *sums* of coefficients found to vanish for the macroscopic steady state. $\rho$ open represents the probability of every conceivable path of the electron, and we expect it to strongly exhibit correlations (memory effects). We interpret the vanishing of $A_3$, $B_3$, $H_3$ when we solve for $\rho$ closed as indicating that in the steady-state the lattice dynamics and the interacting macroscopic electron distribution both maintain their integrity, and not all the available correlation is called for. When the electron is starting out, or if fine grained fluctuations are of interest, then on a physical basis we expect that non-Markovian aspects will play a more obvious part. We also note that if a strong electric field were applied, so that a steady-state condition would never set in, this situation would make itself felt during the formative stage of the electron's evolution. This stage we have not investigated, but rather taken for granted as leading to steady state. With the vanishing of $A_3$, $B_3$, $H_3$ we easily arrive at the goal of our calculation, an explicit form for $\rho$ closed. Equations (6.6) are readily amenable to calculations even with more detailed models of various semiconductors than we have so far been able to consider.

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## APPENDIX A

To lend plausibility to our treatment of the double-path integral in Sec. II, we here use the same approach to derive the Schrödinger equation for the one-dimensional propagator $K$, starting with Feynman's path-integral expression. We recall that if at $t=0$ a particle has a wave function $\psi(R_0,0)$, then at time $t$ its wave function is given by

$$\psi(R_N,t)\equiv\int_{-\infty}^{\infty}K(R_N,R_0;t)\psi(R_0,0)dR_0 \tag{A1}$$

and that then $K(R_N,R_0,t)$ is given by[12]

$$K(R_N,R_0;t)=\int_{R_0}^{R_N}\exp\left[\frac{i}{\hbar}\int_0^t L(\dot{R},R,t')\right]\mathscr{D}R(t') \tag{A2}$$

$$\equiv\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{I=1}^{N}K_I dR_{N-1}\cdots dR_1 \tag{A3a}$$

$$K_I=\left[\frac{ih\tau_I}{m}\right]^{-1/2}\exp\left\{\frac{i\tau_I}{\hbar}\left[\frac{m}{2}\left[\frac{R_I-R_{I-1}}{\tau_I}\right]^2-V(R_I)\right]\right\} \tag{A3b}$$

The time intervals $\tau_I=t_I-t_{I-1}$ are usually taken equal, and, further, the presumption is made that if we take enough time intervals, $K(R_N,R_0,t)$ will approach a limit, the path integral. In our work we treat the $\tau_I$ as independent, but likewise make the assumption that a limit is approached if all $\tau_I$ go to zero.

To derive the Schrödinger equation, Feynman and Hibbs add one more time interval and one more integration, thereby achieving an increase of from $t$ to $t+\tau_N$, or to $(t+dt)$ in the overall time of propagation.[12] This approach of integrating once more is not useful for us, because ultimately we are interested not in $K(R_N,R_0;t)$, $K$ closed, but in $\pi K_I$, $K$ open. Further, we cannot change the number of variables of integration when we change the overall propagation time, since we are doing a problem in $N$ variables, $N$ fixed. For this reason we take the $\tau_I$ as adjustable. However, since we expect to approach the same limit for $K$ closed, and $t=\sum\tau_I$, the Schrödinger equation ought to emerge if we formally differentiate Eq. (A3b) with respect to $\tau_N$ (under the integral sign) keeping the other $\tau$'s fixed. Furthermore, to find the $N$-variable propagator, (the open problem), in general we need more than one differential equation, we need $N$ differential equations. These we get by differentiating with respect to the $N$ variables $\tau_I\cdots\tau_N$, each in turn.

Checking, we find

$$i\hbar\frac{\partial K_N}{\partial\tau_N}=\left[\frac{-i\hbar}{2\tau_N}+\frac{m}{2}\left[\frac{R_N-R_{N-1}}{\tau_N}\right]^2+V(R_N)\right]K_N\ . \tag{A4}$$

We also note that

$$\frac{-\hbar^2}{2m}\frac{\partial^2K_N}{\partial R_N^2}=\left[\frac{m}{2}\left[\frac{R_N-R_{N-1}}{\tau_N}\right]^2-\frac{i\hbar}{2\tau_N}\right]K_N\ . \tag{A5}$$

So, finally

$$i\hbar\frac{\partial K(R_N,R_0;t)}{\partial t}=i\hbar\frac{\partial K(R_N,R_0;t)}{\partial\tau_N}$$
$$=\frac{-\hbar^2}{2m}\frac{\partial^2K(R_N,R_0;t)}{\partial^2R_N^2}+VK(R_N,R_0;t)\ . \tag{A6}$$

## APPENDIX B

In this appendix we reduce the right-hand side of the equation of motion, Eq. (2.3), to where its Fourier transform is a quadratic polynomial in wave vector times the transform of $\rho$ open (which latter factor ultimately cancels from the equation of motion). Let us start with a typical term on the right side of Eq. (2.3), namely

$$T_{NJ}\equiv\exp[i\vec{K}\cdot(\vec{R}_N-\vec{R}_J)]\rho(R_N,R_N',\ldots,R_0,R_0';\tau)\ . \tag{B1}$$

From Eq. (3.9) the transformed term becomes

$$(T_{NJ})_W=\delta\left[\sum \delta\vec{P}_I-\vec{P}_N\right]\delta\left[\sum \delta\vec{u}_I \exp\left[-\sum_{I+1}^{N}\tau_{I'}\right]-\vec{u}_N\right]\exp[i\vec{K}\cdot(\vec{r}_N-\vec{r}_J)]$$

$$\times\left[\frac{m}{h}\right]^{3N}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\frac{im}{\hbar}\vec{y}_N\cdot\vec{u}_N\exp\frac{im}{\hbar}\sum_{I=1}^{N-1}(\vec{u}_I^{+}\cdot\vec{y}'_I-\vec{u}_I^{-}\cdot\vec{y}_I)\exp\frac{-i\vec{K}}{2}\cdot(\vec{y}_N+\vec{y}'_J)$$

$$\times\rho(\vec{r}_N,\ldots,\vec{r}_1;\vec{y}_N,\ldots,\vec{y}_1;\vec{y}'_{N-1},\ldots,\vec{y}'_1;\tau)d^3y_N\cdots d^3y_1 d^3y'_N\cdots d^3y'_1\ . \tag{B2}$$

We now compare the right-hand side of Eqs. (3.7) and (3.9a) but imagine that the $\delta\vec{u}_I$ in $\exp(-i\vec{k}\cdot\delta\vec{u})$ in Eq. (3.9a) are written in terms of the $\vec{u}_I$, as in Eqs. (3.6c). [However, we do not alter the $\delta$ function, which is present in both equations, or, alternately, if we want to be completely formal we can also Fourier represent the $\delta$ function in Eqs. (3.9) and (B2), and proceed from there.] The comparison reveals that if while Wigner transforming, an additional factor $\exp(-i\vec{K}\cdot\vec{y}'_J)$ is introduced, as in Eq. (B2), it causes a shift in $\delta\vec{u}_{J+1}$, but not in $\delta\vec{u}_J$. We summarize

$$(T_{NJ})_W=\exp i\vec{K}\cdot(\vec{r}_N-\vec{r}_J)\rho_W(\vec{r}_N,\vec{u}_N;\delta\vec{r}_N,\ldots,\vec{\delta}_1;\delta\vec{u}_N-\frac{\hbar\vec{K}}{2m}\ ,$$

$$\times\delta\vec{u}_{N-1},\ldots,\delta\vec{u}_{J+2},\delta\vec{u}_{J+1}+\frac{\hbar K}{2m}e^{-\tau_{J+1}},\delta\vec{u}_J,\ldots,\delta\vec{u}_1;\tau)\ . \tag{B3}$$

The other three terms occurring in Eq. (2.2d) for $V_{1,2}(N,J)$ will likewise lead to unequivocal recoils in the $\delta\vec{u}$ coordinates of $\rho_W$ open, as well as again to the factor $\exp[i\vec{K}\cdot(\vec{r}_N-\vec{r}_J)]$.

When now we combine Eq. (B3) for $(T_{NJ})_W$ with the Fourier representation of $\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\vec{u};\tau)$ given in Eq. (3.6a), we see that the recoils represented in Eq. (B3) get translated into exponential factors, where the exponents are wave vectors multiplied into the recoils. The prefactors will be the same as in I. Dropping the prefactors, we are left with

$$\exp i\vec{K}\cdot(\vec{r}_N-\vec{r}_J)\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\tilde{\vec{u}};\tau)\equiv(M_{NJ})_W\ . \tag{B4}$$

The task is to find the Fourier representation of $(M_{NJ})_W$ for ready comparison with the left-hand side of the ID equation. We draw on the Fourier representation of $\rho_W(\vec{P}_N,\vec{u}_N;\vec{P},\delta\vec{u};\tau)$ in Eqs. (4.2). Some algebra then reveals that

$$(M_{NJ})_W=\delta(\Delta\vec{P})\delta(\Delta\tilde{\vec{u}})(2\pi)^{-6N}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp i\vec{K}\cdot\sum_{J+1}^{N}(\delta\vec{P}_I-\vec{u}_{I+}\vec{u}_{I-1})e^{i\vec{K}\cdot(\vec{r}_N-\vec{r}_J)}e^{i\vec{w}\cdot\delta\vec{P}}$$

$$\times e^{i\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}}}\exp[-F(\vec{w},\tilde{\vec{k}};\tau)/2]d^3w\,d^3\tilde{k}$$

$$=\delta(\Delta\vec{P})\delta(\Delta\tilde{\vec{u}})(2\pi)^{-6N}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}e^{i\vec{\omega}\cdot\delta\vec{P}}e^{i\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}}}\exp[-F(\vec{w}^{J},\tilde{\vec{k}}^{J};\tau)/2]d^3w\,d^3\tilde{k}\ , \tag{B5a}$$

where

$$\delta(\Delta\vec{P})\equiv\delta\left[\sum_I\delta\vec{P}_I-\vec{P}_N\right]\ , \tag{B5b}$$

$$\delta(\Delta\tilde{\vec{u}})\equiv\delta\left[\sum_I\delta\tilde{\vec{u}}_I-\vec{u}_N\right]\ , \tag{B5c}$$

and

$$\tilde{\vec{k}}^{J}_I=\tilde{\vec{k}}_I+\vec{K},\quad \vec{w}^{J}_I=\vec{w}_I-\vec{K},\quad J+1<I\le N \tag{B5d}$$

$$\tilde{\vec{k}}^{J}_I=\tilde{\vec{k}}_I+f_J\vec{K},\quad \vec{w}^{J}_I=\vec{w}_I,\quad 1\le I\le N \tag{B5e}$$

$$f_J\equiv 1-\exp\left[\sum_{J+1}^{N}\tau_I\right]\ . \tag{B5f}$$

Recalling from Sec. IV that we are primarily interested only in the Fourier components $\hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};\tau)$ corresponding to the closed situation, we only evaluate $F(\vec{w}^{J}_c,\vec{k}^{J}_c;\tau)$ where

$$\tilde{\vec{k}}^{J}_{Ic}=\vec{q}+\vec{K},\quad \vec{w}^{J}_{Ic}=\vec{p}-\vec{K},\quad J+1\le I\le N \tag{B6a}$$

$$\tilde{\vec{k}}^{J}_{Ic}=\vec{q}+f_J\vec{K},\quad \vec{w}^{J}_{Ic}=\vec{p},\quad 1\le I\le J\ . \tag{B6b}$$

We then find, with

$$F(\vec{p},\vec{q};\tau)+\vec{K}\cdot\vec{R}_1(J)+K^2R(J)\equiv F(\vec{w}^{J}_c,\tilde{\vec{k}}^{J}_c;\tau)\ , \tag{B6c}$$

that

$$\vec{R}_1(J)=2\tilde{\vec{k}}n(J)-2\vec{w}m(J)\ , \tag{B7}$$

and $R(J)$, $m(J)$, and $n(J)$ are as defined at the beginning of Sec. VI, Eqs. (6.2a)–(6.2c).

As noted we are only interested in solving our ID equation for common wave vectors $\vec{p}$ and $\vec{q}$. Returning to Eqs. (2.2) we see that the right-hand side consists of eight terms. The various terms all have the form of $(T_{NJ})_W$ in Eq. (B3). They differ only in their prefactors. For example, for the term considered in Sec. III, we get

$$(T_{NJ})_W = \exp\left\{ -i(\hbar\vec{K}/2m)\cdot(\vec{q}+\vec{K}) \left[ 1 - \exp\left[ -\sum_{J+1}^{N} \tau_I \right] \right] \right\} (M_{NJ})_W \ . \tag{B8}$$

The factor $(M_{NJ})_W$ as in Eqs. (B4) and (B5) is common to all eight terms. The prefactor, again, originates from Fourier representing $\rho_W$ open with the various recoils attached to $\delta\vec{u}_N$ and $\delta\vec{u}_J$ or $\delta\vec{u}_{J+1}$.

We are interested in representing the right-hand side of the ID equation as an integral over $p$ and $q$ of a Taylor series to second order in $p$ and $q$ multiplying

$$\hat{\rho}_W(\vec{p},\vec{q};\tau)\exp[i(\vec{p}\cdot\delta\vec{P}+\vec{q}\cdot\delta\tilde{\vec{u}})] \ .$$

$(M_{NJ})_W$ contributes

$$\exp[-\tfrac{1}{2}F(\vec{w}_c^{\,J},\tilde{\vec{k}}_c^{\,J};\tau)]\exp[i(\vec{p}\cdot\delta\vec{P}+\vec{q}\cdot\delta\tilde{\vec{u}})] \ ,$$

where

$$\exp[-\tfrac{1}{2}F(\vec{p},\vec{q};\tau)]$$

is just $\hat{\rho}_W(\vec{p},\vec{q};\tau)$. We are left with a factor

$$[1-\vec{K}\cdot\vec{R}_1(J)/2+(\vec{K}\cdot\vec{R}_1)^2/8]\{\exp-[K^2R(J)/2]\} \tag{B9}$$

It is now straightforward to obtain the Taylor expansion in $\vec{p}$ and $\vec{q}$ of the entire right-hand side, exponential prefactors included, the whole calculation proceeding as in I.

## APPENDIX C

Here we give some details for reducing the left-hand side of the ID equation of motion, Eq. (2.3). Again the Fourier transform becomes a quadratic polynomial in wave vectors multiplying the transform of $\rho$ open, (which the latter factor, as noted, cancels in the ID equation). Again, transforming to Wigner functions, we see that the left-hand side of the ID equation reads[6,10]:

$$L_S\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\vec{u};\tau) \equiv \left[ \frac{\partial}{\partial\tau_N} + \vec{u}_N\cdot\vec{\nabla}_{P_N} \right] \bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\vec{u};\tau) \ . \tag{C1}$$

From the derivation in Sec. II of the ID equation we know that $\partial/\partial\tau_N$ is taken at constant $\vec{r}_I$ and $\vec{u}_I$, $I=1,2,\ldots,N$. Expressed in the latter variables, $(\sum \delta\tilde{\vec{u}}_I - \vec{u}_N + \vec{u}_0 e^{-t})$ vanishes. Further, we shall only be interested in solving the ID equation for $\tilde{\vec{k}}_I = \vec{q}$, $1 \le I \le N$, whereby

$$\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}} = \sum_I \vec{q}_I\cdot\delta\vec{u}_I \exp\left[ -\sum_{I+1}^{N} \tau_{I'} \right] \ .$$

Since $q$ does not depend on the $\tau$'s, we only need, neglecting the transient term, $\partial/\partial\tau_n\hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};\tau)$. From Eqs. (4.2b), (4.2c), (4.3c), and (5.1d), we have

$$\frac{\partial}{\partial\tau_N}\hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};\tau) = -\frac{1}{2}\left[ p^2\frac{\partial A(\tau_1,\ldots,\tau_N)}{\partial\tau_N} - 2\vec{p}\cdot\vec{q}\frac{\partial H}{\partial\tau_N} + q^2\frac{\partial B}{\partial\tau_N} \right] \hat{\rho}(\vec{p},\ldots,\vec{p},\vec{q},\ldots,\vec{q};\tau) \ . \tag{C2}$$

As a result of Eq. (5.2) we can now rewrite Eq. (C2) as:

$$\dot{\hat{\rho}}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};t) = -\tfrac{1}{2}[p^2\dot{A}(t) - 2\vec{p}\cdot\vec{q}\dot{H}(t) + q^2\dot{B}(t)]\hat{\rho}(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};t) \ , \tag{C3}$$

where the dots signify differentiation with respect to $t$. Turning to the kinetic energy represented in Eq. (C1), and substituting from Eqs. (4.2a), (4.2b), (B5b), and (B5c) we have

$$\begin{aligned} \vec{u}_N\cdot\vec{\nabla}_{p_N}\bar{\rho}_W(\vec{P}_N,\vec{u}_N;\delta\vec{P},\delta\tilde{\vec{u}};t) &= (2\pi)^{-6N}\delta(\Delta\vec{P})\delta(\Delta\tilde{\vec{u}})i \\ &\quad \times \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \left[ \sum_1^N \delta\vec{u}_I \right] e^{i\vec{w}\cdot\delta\vec{P}} e^{i\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}}} \exp[-F(\vec{w},\tilde{\vec{k}};t)/2] d^3w\, d^3\tilde{k} \\ &= -(2\pi)^{-6N}\delta(\Delta\vec{P})\delta(\Delta\tilde{\vec{u}}) \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \vec{w}_N\cdot\sum_{I=1}^{N}\{\vec{\nabla}_{k_I}\exp[-F(\vec{w},\tilde{\vec{k}};t)/2]\} e^{i\vec{w}\cdot\delta\vec{P}} \\ &\quad \times e^{i\tilde{\vec{k}}\cdot\delta\tilde{\vec{u}}} d^3w\, d^3\tilde{k} \ , \end{aligned} \tag{C4}$$

where we have expressed $\delta\vec{u}_I$ by $(\vec{\nabla}k_I/i)\exp(i\vec{k}\cdot\delta\vec{u})$, and then to get the last line we have used integration by parts with respect to $\vec{k}$. Since $\vec{\nabla}P_N$ is here at constant $\vec{P}_1,\ldots,\vec{P}_{N-1}$, it does not affect $\delta(\Delta\vec{P})$, and, therefore, brings down a factor $i\vec{w}_N$. Further, from Eq. (4.2c) we have,

$$\vec{\nabla}_{k_J}F=-\sum_{I=1}^{J}H_{JI}\vec{w}_I-\sum_{I=J}^{N}H_{IJ}\vec{w}_I+\sum_{I=J}^{N}B_{IJ}\vec{\tilde{k}}_I+\sum_{I=1}^{J}B_{JI}\vec{\tilde{k}}_I$$

and, for

$$\vec{w}_I=\vec{p},\quad 1\le I\le N \tag{C5a}$$

$$\vec{\tilde{k}}=\vec{q},\quad 1\le I\le N \tag{C5b}$$

$$\sum_J\vec{\nabla}_{\vec{k}_J}F=-2\vec{p}H(t)+2\vec{q}B(t) \tag{C5c}$$

using Eq. (5.1e). Finally combining Eqs. (4.2), (B5), (C1), and (C3)–(C5), we get for the left-hand side of the ID equation

$$\left[\frac{\partial}{\partial\tau_N}+\vec{u}_N\cdot\vec{\nabla}_{p_N}\right][(2\pi)^{-6N}\delta(\Delta\vec{P})\delta(\Delta\vec{u})e^{i\vec{p}\cdot\delta\vec{P}}e^{i\vec{q}\cdot\delta\vec{u}}\rho_W(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};t)]$$
$$=-\tfrac{1}{2}\{q^2\dot{B}(t)-2\vec{p}\cdot\vec{q}[B(t)+\dot{H}(t)]+p^2[\dot{A}(t)+2H(t)]\}$$
$$\times[(2\pi)^{-6N}\delta(\Delta\vec{P})\delta(\Delta\vec{u})e^{i\vec{p}\cdot\delta\vec{P}}e^{i\vec{q}\cdot\delta\vec{u}}\rho_W(\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q};t)]\ , \tag{C6}$$

where the large term in the square brackets on each side is the $\vec{p},\ldots,\vec{p};\vec{q},\ldots,\vec{q}$ Fourier component of $\rho_W$ open.

## APPENDIX D

Here we tie up loose ends from Sec. VI. The other two equations complementing Eq. (6.5) are

$$\beta[B(t)+\dot{H}(t)]+[H(t)-B(t)]G_2(e^T-1)=G_1(1+e^{-T})+G_2[A_2+H_2(e^T-1)-B_2e^T] \tag{D1}$$

$$\frac{-\beta}{2}\dot{A}(t)-\beta H(t)+H(t)G_2(e^T-1)=G_1+G_2(A_2+H_2e^T)\ . \tag{D2}$$

With (6.5) these give three coupled, linear, first-order differential equations for $A(t)$, $B(t)$, $H(t)$, with constant coefficients. These must have as the standard solution apart from constants a linear function for $A(t)$ and exponentials for $B(t)$ and $H(t)$. Equations (6.6) is the unique solution satisfying conditions at $t=0$. As regards $R(t,s)$ in the exponentials of Eqs. (6.1d) and (6.1e) and defined in Eq. (6.1h), we assume initially that it depends only on $t$ and $s$ as $R(t-s)$, although ostensibly it depends on $t$ as well. However, when having found the solutions given in Eqs. (6.6) we substitute back into Eq. (6.1h) we find $R$ does indeed depend only on $(t-s)$, see Eq. (7.1). Accordingly, we have a true solution.

The interested reader can check that substituting from Eqs. (5.4a)–(5.4) and (6.6a)–(6.6c) into Eq. (6.5) leads to

$$-\beta b_0e^{-2t}=G_1(e^{-T})-(-2h_0+b_0)G_2(1-e^{-T})$$
$$-b_0e^{-2t}G_2(e^T-1)\ . \tag{D3}$$

Simplifying Eqs. (D1) and (D2) in the way, and equating coefficients of $e^{-2t}$, $e^{-t}$, and constants, yields Eqs. (6.6d)–(6.6g).

## APPENDIX E

We give a plausibility argument to show that our $N$ ID equations for $\rho$ open just suffice to determine the matrices of unknown coefficients. We shall consider a simplified situation, in which $\rho_W$ open depends only on the coordinates $\vec{r}_I$, $N\ge I\ge 1$, and the only unknown coefficients are the $A_{II'}$. Extension to the actual situation will be straightforward.

Let us count the number of "degrees of freedom." We recall that $A_{II'}$ depends on $\tau_I,\tau_{I-1},\ldots,\tau_{I'+1}$. We assume that there is also a constant associated with every coefficient. Let $n_I$ be the overall number of coefficients that depend on $\tau_I$, $[n_I=1+(N-I)(N-I+1)]$. Recalling that there are $(N)(N+1)/2$ coefficients all together, the total number of degrees of freedom, $n_{\text{total}}$, will be given by

$$n_{\text{total}}=\sum_1^N n_I+(N)(N+1)/2\ .$$

We recall that the $I$th ID equation is obtained by differentiating $\rho_W$ open with respect to $\tau_I$. If we looked at the right-hand side of this equation we should see that the influence function is a sum of terms, each of which depends on only one pair of variables $\vec{r}_I-\vec{r}_{I'}$, $N\ge I'\ge 0$, $I'\ne I$. Let us, therefore, make a change of variables as follows:

$$\vec{v}_N=\vec{w}_N\ ,$$
$$\vec{v}_{N-1}=\vec{w}_{N-1}-\vec{w}_N\ ,$$
$$\ldots$$
$$\vec{v}_1=\vec{w}_1-\vec{w}_2\ ,$$

so that

$$\sum_{J=1}^{N} \vec{w}_J\cdot(\vec{r}_J-\vec{r}_{J-1})$$
$$=\sum_{J=1}^{N} \vec{v}_J\cdot(\vec{r}_J-\vec{r}_I)+(\sum_{1}^{N} \vec{v}_J=\vec{w}_1)\cdot(\vec{r}_I-\vec{r}_I) .$$

We now Taylor expand the right-hand side of the ID equation in the $v_{I'}$. We then shall get only $(N)$ diagonal terms multiplying $w_1^2, v_1^2, \ldots, v_{I'}^2, \ldots, v_N^2$, respectively, with the $v_I^2$ term missing. If all pairs $v_I v_{I'}$ turned up we would have had $N(N+1)/2$ terms. We recall that solving an ID equation in the limit of small wave vectors just entails setting the final polynomials in the $w$'s, i.e., the polynomials incorporating both sides of the equation, identically equal to zero for all values of all $w_I$. Each polynomial coefficient is a linear function of the $A_{II'}$. Thus, the vanishing of each of the above diagonal terms introduces one new linear relationship among the $A_{II'}$. This is true even though we replace the $v_I$'s by their equivalent $w$'s. When we consider all ID equations, $I=1,2,\ldots,N$, the right-hand sides will contribute one linear relationship for every physical interaction, (every pair), a total of $(N+1)(N)/2$ relationships.

Turning to the left side of the ID equation we recall that $A_{II'}$ has $(I\text{-}I')$ degrees of freedom, since it depends on $\tau_I, \tau_{I-1}, \ldots, \tau_{I'}+1$. Differentiating with respect to $\tau_I$, therefore, introduces $n_I$ relationships. Thus, the total number of relationships is just $n_{\text{total}}$.


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[13]Strictly the contributions to Eqs. (6.5), (D1), and (D2) coming from $K<1$ need special treatment. However, even here no divergences (such as $e^t$, etc.) occur. Since, for deformation-potential coupling integrands typically contain factors of $K^4$, and the important contributions come at $K\sim100$, see I, we are not pursuing the question. Ultimately we are planning to look at polar coupling, where, conceivably, an appreciable correction might result. Nowadays one also makes measurements on submicron samples, where phonon modes $K<1$ do not exist.