

Universal features in degenerate and nondegenerate hot-carrier screening

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The quantum-transport-equation approach, which was used to calculate nonequilibrium screening in the nondegenerate regime [Phys. Rev. B **39**, 8468 (1989)], is extended to study nonequilibrium screening in the highly degenerate regime. We obtain an expression for the nonequilibrium electric susceptibility $\chi(\mathbf{q}, \omega) = \delta n(\mathbf{q}, \omega) / \delta U(\mathbf{q}, \omega)$ for a degenerate system in the presence of a large static electric field, within the relaxation-time approximation. Using the drift-diffusion equation as modified by Thornber and Price to include gradients of the field, we show that in both degenerate and nondegenerate systems, when the drift velocity exceeds a critical velocity v_c ($v_c = v_F / \sqrt{6}$ and $v_c = \sqrt{k_B T / 2m}$ for the degenerate and nondegenerate cases, respectively), the real part of $\chi(\mathbf{q}, \omega = 0)$ is *positive* for small q . The fact that $\text{Re}[\chi(\mathbf{q}, \omega = 0)] > 0$ suggests that, with the proper device configuration, instabilities with respect to density perturbations might be possible. Since the large- q limit of the nonequilibrium χ is the nonequilibrium Lindhard form of the susceptibility, χ_{NL} , we scale χ by χ_{NL} . The ratio $\chi(q) / \chi_{\text{NL}}(q)$ is a *universal* function, independent of both the degeneracy and the value of $mv_c^2 \tau / \hbar$ (the product of the wave vector and mean free path of a carrier with velocity v_c), for $0 < v_d / v_c \lesssim 5$ and $mv_c^2 \tau / \hbar \gtrsim \max\{1, v_d / v_c\}$.

I. INTRODUCTION

The constantly shrinking physical proportions of solid-state devices gives rise to very high operating electric fields within the devices. These fields lead to a highly nonequilibrium distribution of hot carriers, and therefore the study and understanding of the physics of the carriers under nonequilibrium conditions is technologically important. One aspect of the physics that changes in these highly nonequilibrium situations is that of the free-carrier screening. Study of screening is important because it affects the carrier scattering rates and hence the mobilities and distribution function of the carriers. Furthermore, the properties of the collective modes of the free carriers are also altered by changes in the screening.

Various attempts have been made to characterize screening in nonequilibrium situations.¹⁻⁵ Recently, a method by which screening in steady-state nonequilibrium situations can be studied was introduced.^{6,7} In these studies, linear screening in a nondegenerate semiconductor under application of a high electric field was studied, within the relaxation-time approximation for the scattering term. In this paper, we extend the calculation to the case of linear screening in a degenerate electron gas in a high electric field, again within the relaxation-time approximation. Such situations can exist experimentally, for example, in metals or highly doped semiconductors at low temperatures, under application of a high electric field.⁸

Linear screening is quantified by the electric susceptibility $\chi(\mathbf{q}, \omega)$ which is the ratio of the linear density response to the total potential. It has been previously

shown⁶ that the features of the susceptibility in the small- q and $-\omega$ regimes can be understood to first order in q and ω from the conventional drift-diffusion equation [i.e., $\mathbf{j} = n\mathbf{v}_d(\mathbf{F}) - \hat{D}\nabla n$]. However, the conventional drift-diffusion equation did not correctly give the real part of the nonequilibrium static susceptibility at small q . In this paper, we obtain the correct nonequilibrium static susceptibility at small q by using a modification of the drift-diffusion equation that was first introduced by Thornber⁹ to describe velocity overshoot in submicron devices. This modified drift-diffusion equation was subsequently studied by Price¹⁰ and is further generalized in this paper.

Using this modified drift-diffusion equation, we show that the real part of $\chi(\mathbf{q}, \omega = 0)$ is *positive* at $q \sim 0$ for drift velocities that exceed a critical velocity v_c for both the degenerate and nondegenerate systems. Since $\text{Re}(\chi) > 0$ means that the carriers move towards the crest (rather than the trough) of the potential, it implies that, with the proper device configuration, the system could be unstable with respect to density perturbations. Furthermore, the critical velocity v_c provides a convenient velocity scale which permits comparisons to be made between the degenerate and nondegenerate susceptibilities. In the large- q region, both the susceptibilities tend towards the nonequilibrium Lindhard forms of the susceptibility χ_{NL} , in which the equilibrium distribution functions $f_{\text{eq}}(\mathbf{p})$ in the expression for the Lindhard susceptibility are replaced by the nonequilibrium distribution functions. If we scale the actual nonequilibrium static susceptibilities by the nonequilibrium Lindhard susceptibility over the entire range of q , scale the drift velocities by v_c , and scale q by $1/v_c \tau$, we find that the curves obtained in this

manner for the degenerate and nondegenerate systems are quantitatively very similar. This seems to indicate that the scaled nonequilibrium χ 's are independent of the degeneracy of the system, which would simplify the extrapolation of nonequilibrium screening from the highly degenerate to the nondegenerate regime. Moreover, with this scaling procedure, we find that for a given scaled drift velocity, curves for a wide range of scattering rates and Fermi or thermal velocities are essentially identical.

Section II reviews our method for calculating nonequilibrium screening and the relaxation-time approximation used for the scattering. Within this approximation, the analytic results for the nonequilibrium susceptibility of a degenerate system under application of a large static electric field is shown. Section III shows how the small- q behavior of the nonequilibrium susceptibility for both degenerate and nondegenerate systems can be understood, with a modified drift-diffusion equation. For both degenerate and nondegenerate systems, when drift velocities exceed the appropriate critical velocities, the real part of the small- q nonequilibrium static susceptibility is positive. We include a brief discussion on the possibility of obtaining instabilities due to the positive real static susceptibility. Section IV shows that when the drift velocities are scaled by this critical velocity and when the nonequilibrium static susceptibilities are scaled by their large- q approximations of χ , the curves that are obtained are very similar. Section V contains a summary of the paper. In Appendix A, we discuss the effective linear scattering operator, which we use in constructing the modified drift-diffusion equation when the scattering operator is nonlinear. Appendix B discusses the properties of the differential mean free path, a quantity which is used to construct the modified drift-diffusion equation. Appendix C gives the details of the derivation of the modified drift-diffusion equation.

II. NONEQUILIBRIUM LINEAR SCREENING

In this section we briefly review the method obtaining the nonequilibrium linear susceptibility from a quantum transport equation.^{6,7} We also review the quantum relaxation-time approximation that makes the solution to this problem analytically tractable.⁷ We then present the expressions for the nonequilibrium susceptibility for a degenerate system in an applied static homogeneous electric field, for a parabolic band within the relaxation-time approximation.

In linear screening is due to the linear response of the charge density $n_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ to a total potential $U_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$. Linear screening can be calculated by using transport equations, such as the classical Boltzmann equation.⁶ However, in order to observe quantum effects arising from the wavelike nature of electrons, a quantum transport equation such as the Kadanoff-Baym equation has to be used.^{7,11} In this paper, the latter approach is utilized. While the quantum approach is somewhat more complicated than the classical approach, it must be used if nonequilibrium effects on inherently quantum effects such as Friedel oscillations are to be seen. The classical result can always be recovered simply by letting \hbar go to zero.

In Ref. 7, the linear charge-density response is calculated from the Wigner distribution function

$$f(\mathbf{p}, \mathbf{x}, T) = \int d\mathbf{r} \exp[-i(\mathbf{r}\cdot\mathbf{p}/\hbar)] \times \langle \psi^\dagger(\mathbf{x} - \frac{1}{2}\mathbf{r}, T) \psi(\mathbf{x} + \frac{1}{2}\mathbf{r}, T) \rangle. \quad (2.1)$$

By using the Kadanoff-Baym approach, the following quantum transport equation for the Wigner function is obtained¹¹

$$\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla}{m} \right] f(\mathbf{p}, \mathbf{x}, T) + i \int d\mathbf{r} \int \frac{d\mathbf{p}'}{(2\pi\hbar)^3} e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} [U_{\text{eff}}(\mathbf{x} + \frac{1}{2}\mathbf{r}, T) - U_{\text{eff}}(\mathbf{x} - \frac{1}{2}\mathbf{r}, T)] f(\mathbf{p}', \mathbf{x}, T) = S[g^<, g^>, \Sigma^<, \Sigma^>], \quad (2.2)$$

where U_{eff} is the sum of the external potential and the Coulomb potential of the carriers, $S[g^<, g^>, \Sigma^<, \Sigma^>]$ is the quantum scattering term, and $\Sigma^<, \Sigma^>$ are the self-energies. (In this paper, ∇ always refer to the *spatial* derivative. Derivatives with respect to momentum are denoted by $\partial/\partial\mathbf{p}$.) This transport equation is the basis for the calculation of nonequilibrium screening. To recapitulate the calculation procedure, it is briefly given as follows: (i) For the nonequilibrium situation being investigated, set up and solve the quantum transport equation to obtain the "unperturbed" Wigner distribution function $f_0(\mathbf{p})$. (ii) Linearly perturb the transport equation with an additional small sinusoidal potential $U_{\text{eff}}(\mathbf{x}, T) = U_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ to produce a response $f_1(\mathbf{p}) e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ in the Wigner function and solve for $f_1(\mathbf{p})$. (iii) Integrate $f_1(\mathbf{p})$ with respect to \mathbf{p} to obtain n_1 .

The ratio n_1/U_1 gives $\chi(\mathbf{q}, \omega)$, and the dielectric constant $\epsilon(\mathbf{q}, \omega) = 1 - 4\pi e^2 \chi(\mathbf{q}, \omega)/q^2$.

Some approximation for the scattering term in the transport equation has to be made in order to solve the problem analytically. The relaxation-time approximation is widely used as a simple (albeit rough) description of scattering processes. In the classical Boltzmann equation, the scattering term in this approximation takes the form

$$S[f](\mathbf{p}, \mathbf{x}) = \frac{f(\mathbf{p}, \mathbf{x}) - f_{\text{eq}}(\mathbf{p}, \mu + \delta\mu(\mathbf{x}))}{\tau}, \quad (2.3a)$$

$$f_{\text{eq}}(\mathbf{p}, \mu + \delta\mu(\mathbf{x})) = \frac{1}{\exp\{\beta[\epsilon(\mathbf{p}) - \mu - \delta\mu(\mathbf{x})]\} + 1}, \quad (2.3b)$$

where $\beta=1/k_B T$, $\epsilon(\mathbf{p})$ is the carrier kinetic energy, and μ is the global chemical potential. $\delta\mu(\mathbf{x})$, the change in the local chemical potential, is determined by local particle conservation

$$\int \frac{d\mathbf{p}}{4\pi^3\hbar} f(\mathbf{p}, \mathbf{x}) = \int \frac{d\mathbf{p}}{4\pi^3\hbar} f_{\text{eq}}(\mathbf{p}, \mu + \delta\mu(\mathbf{x})) . \quad (2.4)$$

Since the classical relaxation-time approximation does not take the wavelike nature of the carriers into account, a quantum analogue of this approximation that can be used in the quantum transport equation must be found. By analogy with the classical relaxation-time approximation [Eq. (2.3)], the quantum approximation models the collisions by a constant-rate relaxation of the (reduced one-particle) density matrix $\hat{\rho}$ to the (reduced one-particle) local equilibrium density matrix^{7,12}

$$\hat{\rho}_{\text{loc eq}} = \frac{1}{\exp[\beta(\hat{\epsilon} - \mu - \delta\hat{\mu})] + 1} . \quad (2.5)$$

Note that the functions $\epsilon(\mathbf{p})$ and $\delta\mu(\mathbf{x})$ in Eq. (2.3b) have been replaced by the operators $\hat{\epsilon}$ and $\delta\hat{\mu}$ which are diagonal in the momentum and coordinate representations, respectively. As in the classical case, $\delta\mu(\mathbf{x}) = \langle \mathbf{x} | \delta\hat{\mu} | \mathbf{x} \rangle$ is obtained from the particle-conserving condition, $\langle \mathbf{x} | \hat{\rho} | \mathbf{x} \rangle = \langle \mathbf{x} | \hat{\rho}_{\text{loc eq}} | \mathbf{x} \rangle$. It can be shown⁷ that within this approximation, a small static density perturbation n_1 of wave vector \mathbf{q} results in a change in the chemical potential $\delta\mu(\mathbf{q})$ of

$$\delta\mu(\mathbf{q}) = - \frac{n_1}{\chi_L(\mathbf{q}, 0)} , \quad (2.6)$$

where χ_L is the equilibrium Lindhard expression for the susceptibility

$$\chi_L(\mathbf{q}, \omega) = \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \frac{f_{\text{eq}}(\mathbf{p} + \hbar\mathbf{q}/2) - f_{\text{eq}}(\mathbf{p} - \hbar\mathbf{q}/2)}{\epsilon(\mathbf{p} + \hbar\mathbf{q}/2) - \epsilon(\mathbf{p} - \hbar\mathbf{q}/2) - \hbar\omega} . \quad (2.7)$$

This result is consistent with the argument that, at equilibrium, the susceptibility is given by the ratio of the change in density and the change in local chemical potential.¹³ Equation (2.6), together with an expansion of $\hat{\rho}_{\text{loc eq}}$, allows us, in the case of small density perturbations, to construct a scattering term which includes the wavelike nature of the carriers.⁷

We treat the problem where the carriers are acted upon by a strong static homogeneous electric field producing a force \mathbf{F}_0 on each carrier, in which case the “unperturbed” transport equation within the relaxation-time approximation is

$$\mathbf{F}_0 \cdot \frac{\partial f_0}{\partial \mathbf{p}} = - \frac{f_0(\mathbf{p}) - f_{\text{eq}}(p)}{\tau} . \quad (2.8)$$

(In this paper, the subscript “0” always refers to quantities in the presence of the static homogeneous electric field.) The result for the linear density response to the total potential, for a parabolic band and with the relaxation time approximation, is⁷

$$\begin{aligned} n_1 \left[1 - \frac{1}{\chi_L(q, 0)} \int_0^\infty \frac{dt}{\tau} \exp \left[- \frac{i\mathbf{F}_0 \cdot \mathbf{q} t^2}{2m} + i\omega t - \frac{t}{\tau} \right] \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \exp \left[-i \frac{t}{m} \mathbf{p} \cdot \mathbf{q} \right] \left[\frac{f_{\text{eq}}(\mathbf{p} + \hbar\mathbf{q}/2) - f_{\text{eq}}(\mathbf{p} - \hbar\mathbf{q}/2)}{\hbar\mathbf{q} \cdot \mathbf{p} / m} \right] \right] \\ = \frac{iU_1}{\hbar} \int_0^\infty dt \exp \left[- \frac{i\mathbf{F}_0 \cdot \mathbf{q} t^2}{2m} + i\omega t - \frac{t}{\tau} \right] \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \exp \left[-i \frac{t}{m} \mathbf{p} \cdot \mathbf{q} \right] [f_0(\mathbf{p} + \hbar\mathbf{q}/2) - f_0(\mathbf{p} - \hbar\mathbf{q}/2)] . \quad (2.9) \end{aligned}$$

In Ref. 7 we evaluated Eq. (2.9) with $f_{\text{eq}}(p)$ equal to the Maxwell-Boltzmann distribution function. In this paper we evaluate Eq. (2.9) with $f_{\text{eq}}(p)$ equal to the Fermi-Dirac distribution at zero temperature,

$$f_{\text{eq}}(p) = \Theta(p - p_F) , \quad (2.10)$$

where p_F is the Fermi momentum.

Substituting Eq. (2.10) above into Eq. (2.9), one obtains the following relation

$$\begin{aligned} \frac{n_1}{U_1} \left[1 - \frac{|\chi_L(0, 0)|}{\chi_L(q, 0) q v_F \tau} \int_0^\infty dy \exp \left[- \frac{i\mathbf{w}_d \cdot \bar{\mathbf{q}} y^2}{2\bar{\tau}} + i \frac{\omega\tau}{\bar{\tau}} y - \frac{y}{\bar{\tau}} \right] \right. \\ \times \left[\frac{(\bar{q}/2)^2 - 1}{2} \left\{ \text{ci} \left[\left| 1 + \frac{\bar{q}}{2} \right| y \right] - \text{ci} \left[\left| 1 - \frac{\bar{q}}{2} \right| y \right] \right\} + \frac{1}{2\bar{q}^2 y^2} \left\{ \cos \left[\left| 1 + \frac{\bar{q}}{2} \right| y \right] + \cos \left[\left| 1 - \frac{\bar{q}}{2} \right| y \right] \right\} \right. \\ \left. \left. \pm \frac{1}{2\bar{q}y} \left\{ \left| 1 - \frac{\bar{q}}{2} \right| \sin \left[\left| 1 + \frac{\bar{q}}{2} \right| y \right] + \left| 1 + \frac{\bar{q}}{2} \right| \sin \left[\left| 1 - \frac{\bar{q}}{2} \right| y \right] \right\} \right] \right] \\ = - |\chi_L(0, 0)| \int_0^\infty dy \exp \left[- \frac{i\mathbf{w}_d \cdot \bar{\mathbf{q}} y^2}{2\bar{\tau}} + i \frac{\omega\tau}{\bar{\tau}} y - \frac{y}{\bar{\tau}} \right] \left[\frac{\sin(\bar{q}y) - \bar{q}y \cos(\bar{q}y)}{1 + i\mathbf{w}_d \cdot \bar{\mathbf{q}}y} \right] \frac{2\sin(\bar{q}^2 y/2)}{(\bar{q}y)^3} , \quad (2.11) \end{aligned}$$

where $\mathbf{w}_d = \mathbf{p}_d / p_F = \mathbf{F}_0 \tau / p_F$ is the scaled drift momentum, $\bar{\tau} = p_F^2 \tau / m \hbar$, and $\bar{\mathbf{q}} = \mathbf{q} / q_F$, and the \pm is + for $q < 2q_F$ and

– for $q > 2q_F$. The function $\text{ci}(x)$ is the cosine integral function,¹⁴ and $|\chi_L(0,0)| = (mq_F/\hbar^2\pi^2) = (3n_0/mv_F^2)$ is the magnitude of the equilibrium long-wavelength static Lindhard expression for a metal (n_0 is the carrier density). The susceptibility $\chi = n_1/U_1$ can be obtained from this equation.

In the limit where $\hbar \rightarrow 0$, the above equation reduces to one which can be obtained from the classical Boltzmann equation.⁶ The equation is

$$\frac{n_1}{U_1} \left[1 - \int_0^\infty \frac{dx}{s} \frac{\sin x}{x} \exp \left[-\frac{i\mathbf{w}_d \cdot \hat{\mathbf{s}} x^2}{2s} + i\frac{\omega\tau x}{s} - \frac{x}{s} \right] \right] \\ = -|\chi_L(0,0)| \int_0^\infty dx \exp \left[-\frac{i\mathbf{w}_d \cdot \hat{\mathbf{s}} x^2}{2s} + i\frac{\omega\tau x}{s} - \frac{x}{s} \right] \frac{\sin x - x \cos x}{1 + ix\hat{\mathbf{s}} \cdot \mathbf{w}_d} \frac{1}{x^2}, \quad (2.12)$$

where $\mathbf{s} = \mathbf{q}v_F\tau$, and $\hat{\mathbf{s}}$ is the unit vector in the \mathbf{s} direction.

Since these equations are somewhat complicated, it would be advantageous to understand them in certain limits. In the large- q limit, when the effects of the scattering and of the homogeneous electric field \mathbf{F}_0 are negligible over the period of a wavelength, we have shown that the susceptibility approaches the nonequilibrium Lindhard form (which is appropriate for ballistic carriers in the absence of a homogeneous field).^{6,7} In the small- q and $-\omega$ regime, one would expect that hydrodynamic-type equations should describe the screening.¹⁵ Here, one would expect the conventional drift-diffusion equation (i.e., $\mathbf{j} = n\mathbf{v}_d(\mathbf{F}) - \hat{D}\nabla n$) would completely describe the small- q and $-\omega$ regime, but this is not correct. As shown below, a slight modification to the conventional drift-diffusion equation is needed in order to completely describe the nonequilibrium $\chi(\mathbf{q},\omega)$ in this regime.

III. QUASISTATIC SUSCEPTIBILITY AT SMALL WAVE VECTOR: CRITICAL VELOCITIES

In this section, we first note that the conventional drift-diffusion equation does not fully describe the nonequilibrium static susceptibility at small q . We then show that the drift-diffusion equation as modified by Thornber⁹ and Price,¹⁰ and further generalized here to include the effects of degeneracy (henceforth referred to as the Thornber-Price drift-diffusion equation), fully describes the behavior of $\chi(q,0)$ at small q . The Thornber-Price drift-diffusion equation is derived in the appendices using the Boltzmann equation.¹⁶ Then, using this Thornber-Price drift-diffusion equation, we show that within the relaxation-time approximation, the real part of the nonequilibrium static susceptibility is *positive* for small q for drift velocities greater than a critical drift velocity v_c . This critical velocity is $v_F/\sqrt{6}$ for degenerate systems and $\sqrt{k_B T/2m}$ for nondegenerate systems, and provides a convenient velocity scale for making comparisons of the susceptibilities of degenerate and nondegenerate systems.

Figure 1 of Ref. 6 shows that, at small wave vectors and in quasistatic situations, the susceptibility can, to first order in q and ω , be described by the conventional drift-diffusion equation. However, we also saw that the conventional drift-diffusion equation did *not* exactly reproduce the real part of the static susceptibility and that another term was needed in the drift-diffusion equa-

tion to achieve agreement with the results obtained via the Boltzmann equation. The correction to the drift-diffusion equation was introduced phenomenologically by Thornber⁹ and was subsequently derived from the Boltzmann equation by Price.¹⁰

Price showed that for carriers in a homogeneous static electric field producing a force \mathbf{F}_0 , when there is no carrier-carrier interaction and no degeneracy effects in the scattering term, one can write down an *exact* relation for the static linear response of the drift velocity $\delta\mathbf{u}(\mathbf{x})$ to a force perturbation $\delta\mathbf{F}(\mathbf{x})$, and spatial gradients of the density $\nabla n(\mathbf{x})$ and distribution function $\nabla f(\mathbf{p},\mathbf{x})$.¹⁰ The terms that depend on $\delta\mathbf{F}$ and ∇n are the drift and diffusion terms of the conventional drift-diffusion equation, respectively. The third term, which depends on ∇f , is the correction to the drift-diffusion equation.

We review the formulation and extend it to include temporal variations and the possibility of a *nonlinear* scattering operator, so that we can use it to calculate screening in both nondegenerate and degenerate systems. In dealing with small variations in the distribution function around the steady-state distribution function in systems where the scattering operator is nonlinear, we find it convenient to define a linearized scattering operator S_{lin} . S_{lin} is described in the next subsection and in Appendix A.

A. Linearized scattering operator S_{lin}

In a nondegenerate system, the scattering operator S is a *linear* operator. Therefore, when the distribution function deviates from $f_0(\mathbf{p})$ by $\delta f(\mathbf{p})$, the scattering operator changes linearly with $\delta f(\mathbf{p})$

$$S[f_0 + \delta f] - S[f_0] = S[\delta f](\mathbf{p}). \quad (3.1)$$

When the system is degenerate, or when carrier-carrier scattering is present, the scattering operator is *not* linear in $f(\mathbf{p})$. However, if the deviations $\delta f(\mathbf{p})$ of the distribution function from $f_0(\mathbf{p})$ are small, one can linearize the scattering operator around the steady-state $f_0(\mathbf{p})$.¹⁷ Then, the change in the scattering operator due to a small deviation $\delta f(\mathbf{p})$ away from $f_0(\mathbf{p})$, is given by

$$S[f_0 + \delta f] - S[f_0] \approx S_{\text{lin}}[\delta f](\mathbf{p}), \quad (3.2)$$

where S_{lin} is a *linear* operator. Details and examples are given in Appendix A.

B. Differential mean free path $l'(\mathbf{p})$

In the equation that Price obtained relating $\delta\mathbf{u}$ to $\delta\mathbf{F}$, ∇n and ∇f ,¹⁸ the coefficients multiplying $\delta\mathbf{F}$, ∇n and ∇f , all depend on a quantity which Price calls the “differential mean free path”, $l'(\mathbf{p})$. All the coefficients in the Thornber-Price drift-diffusion equation that we obtain below depend on $l'(\mathbf{p})$. In this subsection, we describe the physical meaning of $l'(\mathbf{p})$ when the scattering operator is *linear*. [A nonlinear scattering operator complicates the interpretation of $l'(\mathbf{p})$ a little (see Appendix B).]

The “differential mean free path” $l'(\mathbf{p})$ (in the case where the scattering operator is linear) is the nonequilibrium generalization of the equilibrium concept of the mean free path, $l(\mathbf{p})$. The equilibrium mean free path $l(\mathbf{p})$ is the average distance that a particle with initial momentum \mathbf{p} moves relative to the lattice before it thermalizes. That is,

$$l(\mathbf{p}) = \int_0^\infty dt \overline{v(t)}, \quad (3.3)$$

where $v(t)$ is the velocity of a single particle which had momentum \mathbf{p} at $t=0$, and where the long overbar denotes averaging over many of these particles.

When a static electric field \mathbf{F}_0 is applied, the carriers drift with an average velocity $\mathbf{v}_d(\mathbf{F}_0)$. For this system, the mean free path as defined in Eq. (3.3) will be infinite,

since $\overline{v(t)}$ approaches \mathbf{v}_d as $t \rightarrow \infty$. To define an equivalent finite “mean free path” for a carrier in the presence of a static electric field, the overall drift of the carriers must be subtracted out; therefore, one defines the “differential mean free path”, viz.

$$l'(\mathbf{p}) = \int_0^\infty dt \overline{v(t) - \mathbf{v}_d}. \quad (3.4)$$

Hence, $l'(\mathbf{p})$ is the *difference* between the average distance that a particle with momentum \mathbf{p} moves and the distance that the system as a whole drifts. In other words, $l'(\mathbf{p})$ is the mean free path of a particle with momentum \mathbf{p} in the reference frame that is drifting at velocity \mathbf{v}_d .

In Appendix B, we give a mathematical definition of $l'(\mathbf{p})$ and discuss the interpretation of $l'(\mathbf{p})$ when the scattering operator is nonlinear.

C. Beyond the conventional drift-diffusion approximation: The Thornber-Price drift-diffusion equation

The linear-order change in the drift velocity $\delta\mathbf{u}$ in response to a small (spatially and temporally dependent) change in the force term of the Boltzmann equation is (see Appendix C)

$$\begin{aligned} \delta\mathbf{u}(\mathbf{x}, t) = & \delta\mathbf{F}(\mathbf{x}, t) \cdot \int \frac{\partial}{\partial \mathbf{p}} l'(\mathbf{p}) g_0(\mathbf{p}) d\mathbf{p} - \frac{\nabla n(\mathbf{x}, t)}{n_0} \cdot \int \mathbf{v}(\mathbf{p}) l'(\mathbf{p}) g_0(\mathbf{p}) d\mathbf{p} - \int \nabla g(\mathbf{p}, \mathbf{x}, t) \cdot \mathbf{v}(\mathbf{p}) l'(\mathbf{p}) d\mathbf{p} \\ & - \frac{1}{n_0} \frac{\partial n(\mathbf{x}, t)}{\partial t} \int l'(\mathbf{p}) g_0(\mathbf{p}) d\mathbf{p} - \int l'(\mathbf{p}) \frac{\partial g}{\partial t}(\mathbf{p}, \mathbf{x}, t) d\mathbf{p} + \frac{\delta n}{n_0} \int S_{\text{lin}}[g_0](\mathbf{p}) l'(\mathbf{p}) d\mathbf{p}, \end{aligned} \quad (3.5)$$

where $g(\mathbf{p}, \mathbf{x}, t) = f(\mathbf{p}, \mathbf{x}, t)/n(\mathbf{x}, t)$, is the distribution function normalized by the local density and $g_0(\mathbf{p})$ is the normalized steady-state distribution function in the presence of the static electric field.

To linear order, Eq. (3.5) is exact, but unless one solves for the perturbed transport equation, the terms ∇g and $\partial g/\partial t$ are unknown. A further approximation would be to assume

$$\begin{aligned} \nabla g &= \nabla \mathbf{F} \cdot \frac{\partial g_0}{\partial \mathbf{F}} + \nabla n \frac{\partial g_0}{\partial n}, \\ \frac{\partial g}{\partial t} &= \frac{\partial \mathbf{F}}{\partial t} \cdot \frac{\partial g_0}{\partial \mathbf{F}} + \frac{\partial n}{\partial t} \frac{\partial g_0}{\partial n}, \end{aligned} \quad (3.6)$$

where the derivatives with respect to \mathbf{F} and n are evaluated at \mathbf{F}_0 and n_0 , respectively. This would clearly be valid only in the small wave vector (e.g., $qv_F\tau$, $qv_d\tau \lesssim 1$ in the degenerate case) and quasistatic ($\omega\tau \lesssim 1$) regime, since it assumes that the distribution function at any point \mathbf{x} is dependent only on the local density $n(\mathbf{x})$ and the local electric force $\mathbf{F}(\mathbf{x})$. Using these approximations in Eqs. (3.6), and the result [see Appendix B, Eq. (B19)]

$$\int l'(\mathbf{p}) \left[\frac{g_0(\mathbf{p})}{n_0} + \frac{\partial g_0}{\partial n}(\mathbf{p}) \right] d\mathbf{p} \equiv \int l'(\mathbf{p}) \frac{\partial f_0}{\partial n}(\mathbf{p}) d\mathbf{p} = 0, \quad (3.7)$$

Eq. (3.5) becomes

$$\begin{aligned} \delta\mathbf{u} = & \delta\mathbf{F} \cdot \int \frac{\partial}{\partial \mathbf{p}} l' g_0(\mathbf{p}) d\mathbf{p} - \frac{\nabla n}{n_0} \cdot \int \mathbf{v}(\mathbf{p}) l'(\mathbf{p}) \frac{\partial f_0}{\partial n}(\mathbf{p}) d\mathbf{p} \\ & - \sum_{ij} \frac{\partial F_j}{\partial R_i} \int \frac{\partial g_0(\mathbf{p})}{\partial F_j} v_i(\mathbf{p}) l'(\mathbf{p}) d\mathbf{p} \\ & - \frac{\partial \mathbf{F}}{\partial t} \cdot \int l'(\mathbf{p}) \frac{\partial g_0}{\partial \mathbf{F}}(\mathbf{p}) d\mathbf{p} \\ & + \frac{\delta n}{n_0} \int S_{\text{lin}}[g_0](\mathbf{p}) l'(\mathbf{p}) d\mathbf{p}. \end{aligned} \quad (3.8)$$

This is the Thornber-Price drift-diffusion equation. The first two terms are the drift and diffusion terms of the conventional drift-diffusion equation, whereas the other terms are corrections to the drift-diffusion equation which turn out to have important consequences in the behavior of the long-wavelength nonequilibrium susceptibility.

D. The Thornber-Price drift-diffusion equation within the single-rate relaxation-time approximation

In the single-rate relaxation-time approximation in a parabolic band, the differential mean free path is (see Appendix B)

$$l'(\mathbf{p}) = \left[\frac{\mathbf{p}}{m} - \mathbf{v}_d \right] \tau, \quad (3.9)$$

where $\mathbf{v}_d = \mathbf{F}_0 \tau / m$. With this, and the expression for $S_{\text{lin}}[g_0]$ (see Appendix B), all the coefficients of Eq. (3.8) can be calculated. We do this for both the degenerate and nondegenerate systems in a parabolic band, with the electric force vector \mathbf{F}_0 in the z direction ($\hat{\mathbf{x}}_i$ for $i=1,2,3$ are the unit vectors in the $x, y,$ and z directions, respectively)

$$\delta \mathbf{u} = \delta \mathbf{F} \frac{\tau}{m} - \frac{v_d \tau^2}{m} \left[2 \frac{\partial \mathbf{F}}{\partial x_3} + \nabla \cdot \mathbf{F} \hat{\mathbf{x}}_3 \right] - \frac{\tau^2}{m} \frac{\partial \mathbf{F}}{\partial t} - \sum_i \frac{1}{n_0} \frac{\partial n}{\partial x_i} (2v_c^2 + \delta_{i3} v_d^2) \tau \hat{\mathbf{x}}_i, \quad (3.10)$$

where $v_c = v_F / \sqrt{6}$ for the degenerate case and $v_c = \frac{1}{2} v_{\text{th}} = \frac{1}{2} \sqrt{2k_B T / m}$ for the nondegenerate case. We show in the next subsection that v_c corresponds to the drift velocity at which $\text{Re}[\chi(q \sim 0)]$ becomes positive.

We compare Eq. (3.10) with the form [Eq. (3.11)] that Price originally wrote the equation [Eq. (3) of Ref. 10] where the perturbations of field and density were assumed to be only in the direction of \mathbf{F}_0 ,

$$u = u(F_0 + \delta F) \left[1 + \frac{L(F_0)}{F_0} \frac{dF}{dz} \right] - \frac{D(F_0)}{n} \frac{dn}{dz}. \quad (3.11)$$

On comparison of Eqs. (3.10) and (3.11), we see that the field-dependent diffusion coefficient $D(F_0)$ is given by

$$D(F_0) = (2v_c^2 + v_d^2) \tau. \quad (3.12)$$

The longitudinal diffusion constants increase with increasing field because the distribution heats up. Roughly speaking, since the diffusion coefficient is proportional to the effective temperature of the carriers (by the Einstein relation), heating the distribution by increasing the field will increase the diffusion constant.¹⁹

By comparing the field-gradient terms in Eqs. (3.10) and (3.11) we see that the length coefficient defined by Price in Eq. (3.11) is given by

$$L(F_0) = -3 \frac{F_0 \tau^2}{m} = -3 v_d \tau \quad (3.13)$$

in both the degenerate and nondegenerate cases of our calculation. Note that we find $L(F_0)$ to be *negative* within our single-rate relaxation-time approximation. In this approximation, the fact that $L(F_0) < 0$ can be explained by arguing that a small fraction of carriers travel ballistically from regions of higher field to region lower field (see Fig. 1). In contrast, Artaki concluded that the $L(F)$ is *positive* from a Monte Carlo simulation of n -type silicon.²⁰ It is possible that in his simulation, because of problems with obtaining sufficient statistics, Artaki did not go to small enough wave vector and so was probing the regime where the Thornber-Price drift-diffusion equation is not valid.

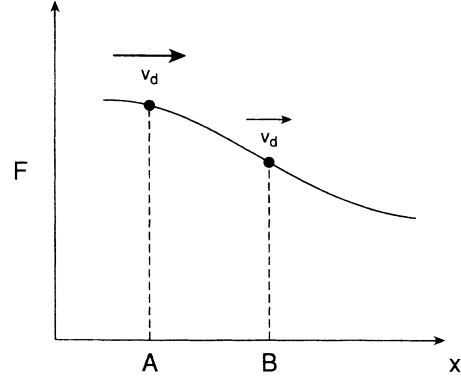


FIG. 1. Explanation of the sign of the length coefficient $L(F_0)$. In a slowly varying inhomogeneous electric field as shown above, the carriers at point A on average have a higher drift velocity than carriers at point B (assuming $dv_d/dF > 0$). A small fraction of the carriers will travel ballistically from A to B . Since these ballistic carriers arriving at B originated from A , a region with a higher drift velocity, their presence should *increase* the average velocity of the carriers at B . Since the change in the average velocity due to the field gradient is given by $[v_d L(F_0)/F_0](dF/dx)$ [cf. Eq. (3.11)], to obtain a positive change with $dF/dx < 0$ (as at point B), $L(F_0)$ must be negative.

E. Possible instabilities

We can use Eq. (3.10), along with the continuity equation $\nabla \cdot \mathbf{j} + \partial n / \partial t = 0$ to calculate the nonequilibrium susceptibility. The expression for $\chi_{\text{TP}}(s, 0)$, the nonequilibrium static susceptibility obtained from the Thornber-Price drift-diffusion equation, is

$$\chi_{\text{TP}}(Q, 0) = -|\chi_L(0, 0)| \left[\frac{Q^2 - 3iQ^3 \bar{w}_d}{iQ\bar{w}_d/2 + (1 + \bar{w}_d^2/2)Q^2} \right], \quad (3.14)$$

where $Q = qv_c \tau$, $\bar{w}_d = \mathbf{v}_d \cdot \hat{\mathbf{Q}} / v_c$ ($\hat{\mathbf{Q}}$ is the unit vector in the \mathbf{Q} direction), and $\chi_L(0, 0) = n_0 / (2mv_c^2)$ is the equilibrium static susceptibility at $q = 0$. The Q^3 term in the numerator of Eq. (3.14) is a direct result of the field-gradient terms of Eq. (3.10). Expanding the denominator of Eq. (3.14) in powers of Q/\bar{w}_d gives (to second order in Q)

$$\chi_{\text{TP}}(Q, 0) = \frac{2|\chi_L(0, 0)|}{\bar{w}_d} \left[iQ + 2Q^2 \left[\bar{w}_d - \frac{1}{\bar{w}_d} \right] \right]. \quad (3.15)$$

This equation is consistent with those obtained from expanding the nonequilibrium susceptibilities derived from the Boltzmann equation [Eq. (2.12) in this paper and Eq. (3) in Ref. 6] in powers of q .

From Eq. (3.15), we see that the sign of the real part of the $\chi_{\text{TP}}(Q, 0)$ goes from *negative* to *positive* when the scaled drift velocity \bar{w}_d exceeds 1. This sign change has two implications. First, this critical velocity v_c ($v_c = v_F / \sqrt{6}$ for the degenerate case and $v_c = v_{\text{th}} / 2 = \sqrt{k_B T / 2m}$ in the nondegenerate case) at which the real part of χ_{TP} becomes positive (at $q \sim 0$) sets a natural velocity scale with which to compare nonequilibrium sus-

ceptibilities of the degenerate and nondegenerate regimes, as discussed in the next section. Second, a positive real part of the susceptibility implies that the carriers tend to move towards the *crest* (rather than the trough) of the potential (recall that the susceptibility is defined by $\chi = n_1/U_1$). Since carriers at the crest of the potential will *enhance* rather than screen the potential, one can speculate that with the proper device design, this system might be coaxed into becoming unstable with respect to small density perturbations, by application of a sufficiently large electric field so that the drift velocity of the carriers exceeds v_c .²¹

Finally, note that a positive real part of the susceptibility in the Eq. (3.15) is due to a sufficiently large *negative* imaginary coefficient of the Q^3 terms in the numerator of Eq. (3.14). The Q^3 term itself, as noted above, is generated by the electric-force-gradient term, while its *negative* imaginary coefficient is due to a *negative* length coefficient $L(F_0)$. Therefore, to produce a region of positive real $\chi_{\text{TP}}(Q,0)$, a sufficiently large negative $L(F_0)$ is required.

IV. SCALED NONEQUILIBRIUM STATIC SUSCEPTIBILITIES FOR DEGENERATE AND NONDEGENERATE SYSTEMS

In the previous section, we showed that the real part of the nonequilibrium static susceptibility at $q \sim 0$ was positive for drift velocities exceeding the critical velocities $v_c = v_F/\sqrt{6}$ and $v_c = v_{\text{th}}/2$ for degenerate and nondegenerate systems, respectively. The v_c for a degenerate or a nondegenerate system provides a natural velocity unit for scaling. In this section, we show that when the nonequilibrium static χ 's are scaled by the nonequilibrium Lindhard expression of susceptibility, χ_{NL} , the velocities are scaled by v_c and the lengths are scaled by $v_c\tau$, the scaled χ 's for the degenerate and nondegenerate systems are remarkably similar.

A. Scaled susceptibility χ/χ_{NL}

The nonequilibrium static susceptibilities in the large- q limit, when the wavelength becomes shorter than the mean free path and the energy gained by carrier over the wavelength is negligible compared to the energy it possesses, tend to the nonequilibrium Lindhard form^{6,7}

$$\chi_{\text{NL}}(\mathbf{q}, \omega=0) = \int \frac{d\mathbf{p}}{4\pi^3 \hbar^3} \frac{f_0(\mathbf{p} + \hbar\mathbf{q}/2) - f_0(\mathbf{p} - \hbar\mathbf{q}/2)}{\hbar\mathbf{q} \cdot \mathbf{p} / m - i0^+}, \quad (4.1)$$

where the $f_0(\mathbf{p})$'s are the *nonequilibrium* distribution functions. Since the true χ approaches χ_{NL} at large q , we divide the true χ by χ_{NL} , so that at large q the scaled susceptibility χ/χ_{NL} approaches unity. A comparison of the scaled curves with the same v_d/v_c , but for different degeneracies and different τ 's, can then be made.

The $\chi(\mathbf{q}, \omega=0)$ are evaluated from the quantum transport equation, i.e., Eq. (2.11) for the degenerate case and Eq. (32) of Ref. 7 for the nondegenerate case, and then divided by their respective χ_{NL} 's. The magnitude and

phase of these scaled curves are plotted as a function of q in Fig. 2 for $v_d = 0.8v_c$ and in Fig. 3 for $v_d = 4v_c$. The wave vector has been scaled by $v_c\tau$, and we show curves with $mv_c^2\tau/\hbar = \infty$ (the classical limit) and $mv_c^2\tau/\hbar = 0.1$. The parameter $mv_c^2\tau/\hbar$ is the product of the wave vector mv_c/\hbar and the mean free path $v_c\tau$ of a carrier with velocity v_c .

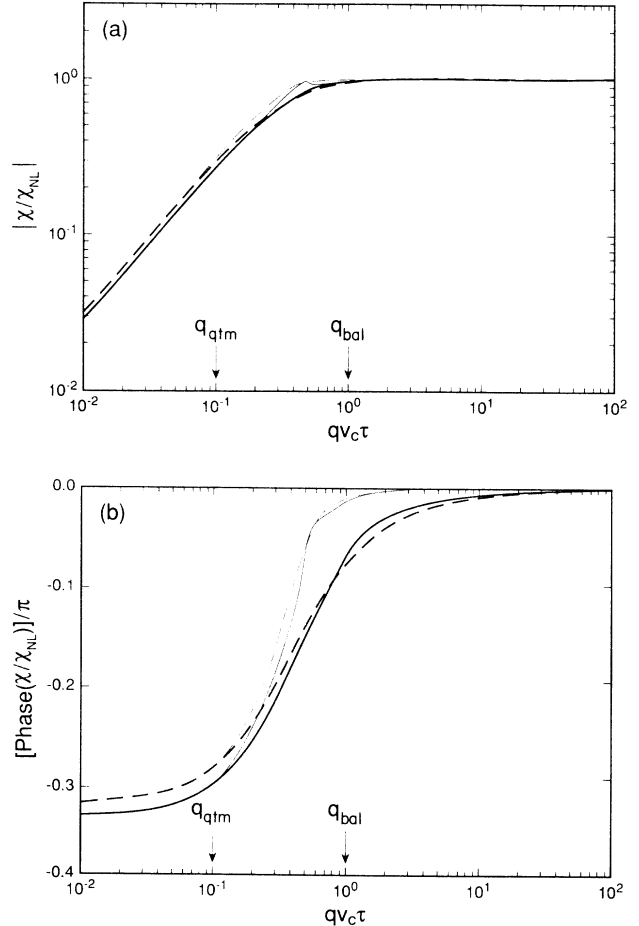


FIG. 2. The ratio of the nonequilibrium static susceptibility $\chi(q, \omega=0)$ (as calculated from the quantum transport equation within the quantum relaxation-time approximation) to the nonequilibrium Lindhard form of the static susceptibility χ_{NL} (where the nonequilibrium $f_0(\mathbf{p})$'s are inserted into the equilibrium form of the Lindhard function), for degenerate and nondegenerate systems, at drift velocity $v_d = 0.8v_c$ {where v_c is the minimum drift velocity at which $\text{Re}[\chi(q \rightarrow 0, \omega=0)]$ is positive}. Since this ratio is a complex quantity, its magnitude of the ratio is shown in (a), and the phase of the ratio is shown in (b). The solid lines are for the degenerate case, and the dashed lines are for the nondegenerate case. The bold-face lines correspond to the classical Boltzmann equation case ($mv_c^2\tau/\hbar = \infty$), while the light-face lines correspond to $mv_c^2\tau/\hbar = 0.1$. The wave vectors $q_{\text{qtm}}v_c\tau \approx mv_c^2\tau/\hbar$ for the $mv_c^2\tau/\hbar = 0.1$ case, and $q_{\text{bal}}v_c\tau \approx \max\{1, v_d/v_c\}$ are indicated. In either case, the curves for these scaled nondegenerate and degenerate susceptibilities are very similar and seem to imply some kind of “universality” of the nonequilibrium χ 's, independent of the degeneracy. Furthermore, *all* curves with $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$ are almost indistinguishable from the classical curve.

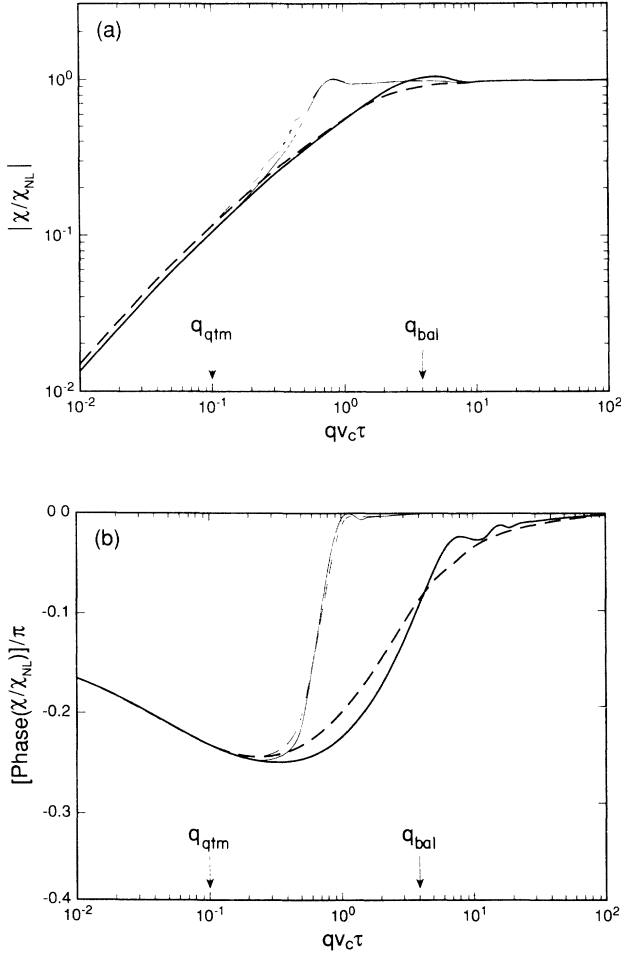


FIG. 3. Same as Fig. 2, except for $v_d = 4v_c$. Again, the solid lines are for the degenerate case and the dashed lines are for the nondegenerate case; and, the bold-face lines correspond to classical Boltzmann curve $mv_c^2\tau/\hbar = \infty$, while the light-face lines correspond to $mv_c^2\tau/\hbar = 0.1$. Again, the curves for the scaled nondegenerate and degenerate susceptibilities are very similar, and all curves for $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$ are almost indistinguishable from the classical curve.

Figures 2 and 3 display the remarkable similarity between the scaled degenerate and nondegenerate static susceptibilities of equal v_d/v_c and $mv_c^2\tau/\hbar$. This similarity persists up to $v_d/v_c \approx 5$, the highest value tested. We speculate that the properly scaled susceptibilities will also be similar for a fermion gas at any temperature (i.e., full degeneracy to nondegenerate regimes).

B. Universality for $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$

In addition, for a given v_d/v_c , all curves of χ/χ_{NL} with $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$ are almost indistinguishable from the classical (i.e., $mv_c^2\tau/\hbar = \infty$) χ/χ_{NL} curve. This indistinguishability means that, over an extremely wide range of scattering rates and thermal or Fermi velocities, the scaled χ/χ_{NL} is equal to a universal curve $(\chi/\chi_{NL})_{univ}$ which is determined *classically*. That is, in $(\chi/\chi_{NL})_{univ}$, the χ is obtained from the *classical*

Boltzmann calculation, and χ_{NL} is the susceptibility for a collisionless *classical* plasma²²

$$\chi(\omega=0) = \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \frac{\hat{\mathbf{q}} \cdot \partial f(\mathbf{p}) / \partial \mathbf{p}}{\hat{\mathbf{q}} \cdot \mathbf{v} - i0^+}, \quad (4.2)$$

which is the classical limit of the nonequilibrium Lindhard susceptibility Eq. (4.1).

The argument for this universality of χ/χ_{NL} for $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$ is as follows. We begin by introducing two characteristic wave vectors (which depend on the system and on the drift velocity), q_{qtm} and q_{bal} . The first of these, q_{qtm} is the largest wave vector at which the classical description of the carriers is valid; that is, for $q > q_{qtm}$, the quantum (i.e., wave) nature of the carriers plays an important role. Hence, for $q < q_{qtm}$, the classical Boltzmann equation and the classical collisionless plasma susceptibility are good approximations for determining χ and χ_{NL} , respectively. This implies that for $q < q_{qtm}$, the scaled χ/χ_{NL} curve is essentially identical to the universal curve $(\chi/\chi_{NL})_{univ}$ [since $(\chi/\chi_{NL})_{univ}$ is given by the classical χ and χ_{NL}]. We show below that in the relaxation-time approximation q_{qtm} is given by the thermal or Fermi momentum. For $q > q_{qtm}$, this argument makes no claim about χ/χ_{NL} ; that is, for $q > q_{qtm}$, χ/χ_{NL} may or may not be universal. The universality of χ/χ_{NL} for large q is determined by the second characteristic wave vector, q_{bal} .

Over short distances, a carrier in a scattering medium under an applied field can be considered to be moving ballistically. The criteria for the validity of approximating the motion of the carrier over some distance by ballistic motion⁶ are that, over that distance (1) there is a low probability that the carrier is scattered and (2) the carrier does not gain a significant amount of energy from the field. For a given system and drift velocity, there is a largest length l_{bal} for which both of the above criteria hold for a typical carrier. For $ql_{bal} > 2\pi$, most carriers move ballistically in the (wave)length $2\pi/q$. Since the nonequilibrium Lindhard χ_{NL} is the susceptibility for ballistic carriers with a distribution $f_0(\mathbf{p})$ (recall in the derivation of the Lindhard susceptibility, the carriers are assumed not to scatter, and there is no applied homogeneous static field²³), then for $ql_{bal} > 2\pi$, $\chi \approx \chi_{NL}$ because most carriers are traveling ballistically over the distance of the wavelength. We define $q_{bal} \approx 2\pi/l_{bal}$. Then, for $q > q_{bal}$, $\chi/\chi_{NL} \approx 1$ for all systems, and hence is universal. Note that for $q < q_{bal}$, this argument makes no claim about χ/χ_{NL} ; that is, for $q < q_{bal}$, χ/χ_{NL} may or may not be universal.

Since the scaled susceptibility χ/χ_{NL} is equal to the universal $(\chi/\chi_{NL})_{univ}$ for $q < q_{qtm}$ and $q > q_{bal}$, it follows that if $q_{bal} < q_{qtm}$, then the scaled curves are equal to $(\chi/\chi_{NL})_{univ}$ for all q . Therefore, the χ/χ_{NL} is universal if $q_{bal} < q_{qtm}$. Below, we give estimates for both q_{bal} and q_{qtm} for the relaxation-time approximation and show that in this approximation $q_{bal} < q_{qtm}$ is equivalent to $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$.

To estimate q_{qtm} , we look at Eq. (2.9), the equation relating the density response to the perturbing potential in

the relaxation-time approximation. The classical limit of Eq. (2.9) is obtained by expanding the distribution functions in powers of $\hbar\mathbf{q}$ and keeping only the first nonvanishing term, i.e.,

$$\begin{aligned} f_{\text{eq}}(\mathbf{p} + \hbar\mathbf{q}/2) - f_{\text{eq}}(\mathbf{p} - \hbar\mathbf{q}/2) &\approx \hbar\mathbf{q} \cdot \frac{\partial f_{\text{eq}}}{\partial \mathbf{p}}, \\ f_0(\mathbf{p} + \hbar\mathbf{q}/2) - f_0(\mathbf{p} - \hbar\mathbf{q}/2) &\approx \hbar\mathbf{q} \cdot \frac{\partial f_0}{\partial \mathbf{p}}. \end{aligned} \quad (4.3)$$

When is this valid? Actually, since these terms are integrated over \mathbf{p} in Eq. (2.9), the real question is, when is it valid to keep only the first term in the expansions of the projections of the distribution functions onto the \mathbf{q} axis

$$F_{\text{eq},0}(p_{\parallel}) = \int \frac{d\mathbf{p}_{\perp}}{4\pi^2\hbar^2} f_{\text{eq},0}(\mathbf{p}_{\perp}, p_{\parallel}), \quad (4.4)$$

(where p_{\perp} and p_{\parallel} are perpendicular and parallel to \mathbf{q} , respectively); that is, when can we approximate

$$\begin{aligned} F_{\text{eq}}(p_{\parallel} + \hbar q/2) - F_{\text{eq}}(p_{\parallel} - \hbar q/2) &\approx \hbar q \frac{dF_{\text{eq}}}{dp_{\parallel}}, \\ F_0(p_{\parallel} + \hbar q/2) - F_0(p_{\parallel} - \hbar q/2) &\approx \hbar q \frac{dF_0}{dp_{\parallel}}. \end{aligned} \quad (4.5)$$

This approximation is valid only if the second- and higher-order terms of the expansion of the projected distribution functions are small, or equivalently, when $\hbar q/p_{F,\text{th}} < 1$ (where p_F and p_{th} are for the degenerate and nondegenerate cases, respectively). Therefore, as long as $q < p_{F,\text{th}}/\hbar$, the classical description is valid. Therefore, q_{qtm} is roughly given by

$$q_{\text{qtm}} \approx p_{F,\text{th}}/\hbar. \quad (4.6)$$

Below, we give a rough estimate for the wave vector q_{bal} at which the criteria for ballistic transport previously given breaks down. The first criterion, that scattering probability is small over the wavelength, is roughly (i.e., ignoring factors of order 1) quantified by

$$qv_{F,\text{th}}\tau \gtrsim 1. \quad (4.7)$$

The second criterion, that the energy gained from the field is small over the wavelength, is roughly given by

$$\frac{F_0}{q} \lesssim mv_{F,\text{th}}^2. \quad (4.8)$$

Substituting $mv_d = F_0\tau$ into Eq. (4.8) gives

$$qv_{F,\text{th}}\tau \gtrsim v_d/v_{F,\text{th}}. \quad (4.9)$$

Since q_{bal} is defined as the wave vector where *both* the above conditions are satisfied, we find

$$q_{\text{bal}}v_{F,\text{th}}\tau \approx \max\{1, v_d/v_{F,\text{th}}\}. \quad (4.10)$$

Equation (4.10) can also be obtained by looking at Eq. (2.12). In Eq. (2.12), if $q > q_{\text{bal}}$, the terms in the exponent corresponding to scattering and acceleration from the field (the $-x/s$ and $-i\mathbf{w}_d \cdot \hat{\mathbf{s}}x^2/2s$ terms, where $\mathbf{w}_d = \mathbf{p}_d/p_F$ and $s = qv_{F,\text{th}}\tau$) are small, and therefore one obtains the susceptibility for ballistic carriers.

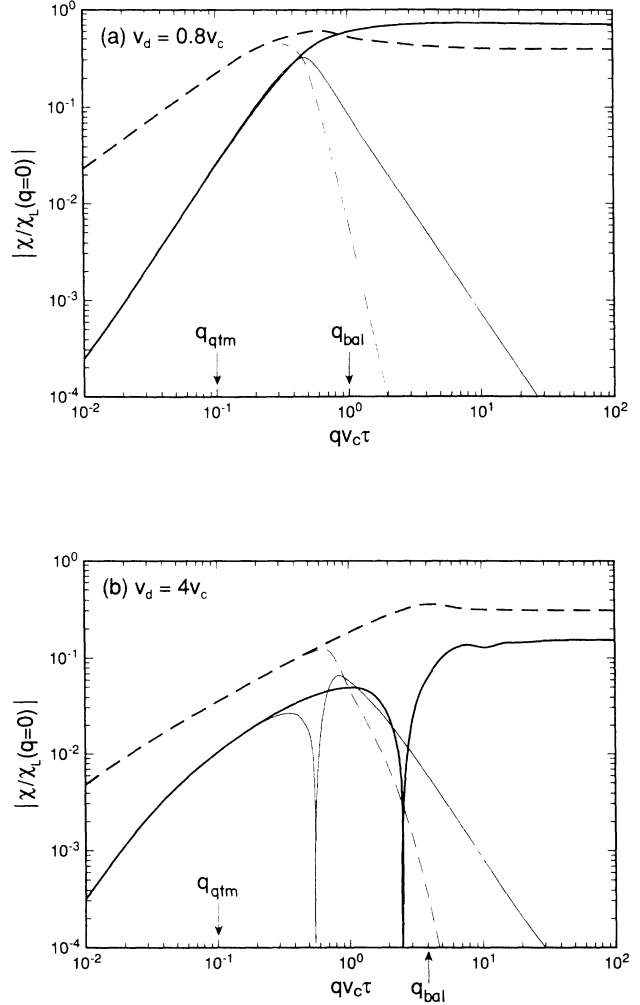


FIG. 4. The imaginary part (dashed lines) and absolute value of the real part (solid lines) of the degenerate, nonequilibrium static susceptibility, $\chi(q, \omega=0)/|\chi_L(0,0)|$ for (a) $v_d = 0.8v_c$ and (b) $v_d = 4v_c$, calculated from the quantum transport equation. The bold-face lines are for the classical Boltzmann case ($mv_c^2\tau/\hbar = \infty$), and the light-face lines are for $mv_c^2\tau/\hbar = 0.1$. For $q \lesssim q_{\text{qtm}}$ (where q_{qtm} is the wave vector at which the classical description breaks down due to quantum effects resulting from the wave nature of the carriers) the $mv_c^2\tau/\hbar = 0.1$ curves are essentially indistinguishable from classical Boltzmann curve. The wave vectors $q_{\text{qtm}}v_c\tau \approx mv_c^2\tau/\hbar$ for the $mv_c^2\tau/\hbar = 0.1$ case, and $q_{\text{bal}}v_c\tau \approx \max\{1, v_d/v_c\}$ are indicated on the figures. For $q > q_{\text{qtm}}$, χ falls off quickly, since it tracks the rapidly decreasing χ_{NL} . In the small- q limit, when $qv_c\tau \lesssim \min\{v_c/v_d, 1/\sqrt{6}\}$ (i.e., the wavelength is much smaller than the equilibrium mean free path, or the drift mean free path) and $q \lesssim q_{\text{qtm}}$ (not in the quantum regime) then one can understand χ from a “hydrodynamic” type of equation (the Thornber-Price drift-diffusion equation). In the large- q regime, when $qv_c\tau \gtrsim q_{\text{bal}}$ (carrier does not scatter or gain significant amount of energy within a wavelength) then the susceptibility approaches the nonequilibrium Lindhard form, which is the susceptibility for collisionless carriers in the absence of a field. Note that in (a), since $v_d < v_c$, the real part is always negative, whereas in (b), since $v_d > v_c$, the real part is positive for small q , and then becomes negative as q increases.

From Eqs. (4.6) and (4.10), we see that the condition for obtaining the universal curve $q_{\text{bal}} < q_{\text{qtm}}$ is given by $mv_{F,\text{th}}^2\tau/\hbar \gtrsim \max\{1, v_d/v_{F,\text{th}}\}$. Since $v_c = v_F/\sqrt{6}$, $v_{\text{th}}/2$, and the arguments given above are only ‘‘order of magnitude’’ type of arguments, we replace $v_{F,\text{th}}$ by v_c , which gives the condition for universality

$$mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}. \quad (4.11)$$

C. Breakdown of universality for $mv_c^2\tau/\hbar < \max\{1, v_d/v_c\}$

We now discuss what happens when the condition for universality fails. We illustrate the behavior of χ/χ_{NL} for $mv_c^2\tau/\hbar < 1$ in Figs. 4(a) and 4(b). In these figures, we show the static susceptibilities (scaled only by the static-equilibrium susceptibility $|\chi_L(q=0)|$, i.e., scaled only by a *real positive constant*) for the degenerate case, for $mv_c^2\tau/\hbar = \infty$ (bold line) and $mv_c^2\tau/\hbar = 0.1$ (thin line), with $v_d = 0.8v_c$ [Fig. 4(a)] and $v_d = 4v_c$ [Fig. 4(b)]. In the scaled wave-vector unit $qv_c\tau$ used for the x axis, the position of the wave vectors q_{qtm} and q_{bal} are given by $q_{\text{qtm}}v_c\tau \approx (mv_c^2\tau/\hbar)$ and $q_{\text{bal}}v_c\tau \approx \max\{1, v_d/v_c\}$. The q_{qtm} for the $mv_c^2\tau/\hbar = 0.1$ case (thin line) and q_{bal} are shown on the figures.

We see that for both the drift velocities shown, the q dependence of the real and imaginary parts of the $mv_c^2\tau/\hbar = 0.1$ curves track the classical limit curve ($mv_c^2\tau/\hbar = \infty$), until approximately q_{qtm} . For $q \gtrsim q_{\text{qtm}}$, the χ for $mv_c^2\tau/\hbar = 0.1$ fall sharply. This behavior of χ for $q \gtrsim q_{\text{qtm}}$ ($\sim q_F$) can be explained by noting that the carriers cannot respond to spatial disturbances for q greater than roughly the diameter of the Fermi surface. The behavior of χ_{NL} as a function of q gives a rough indication of the effect of the diameter of the Fermi surface on χ . For $q \gtrsim q_{\text{qtm}}$, the χ_{NL} decreases, and the true χ tracks it and also decreases for $q \gtrsim q_{\text{qtm}}$. However, the scaled susceptibility χ/χ_{NL} , being the ratio of χ to χ_{NL} , does not decrease. In fact, from Figs. 2 and 3, we see that for $q > q_{\text{qtm}}$, the magnitude scaled susceptibility for $mv_c^2\tau/\hbar = 0.1$ rises *above* the universal curve and then saturates (at 1) at a q lower than q_{bal} (which is where the universal curve saturates). The curves for the phase behave in a similar fashion. At this time, we do not have an explanation for this behavior.

D. Wave-vector range for $\text{Re}(\chi) > 0$

Note that in Fig. 4(a), when $v_d < v_c$, the real part of χ is *always* negative, whereas in Fig. 4(b), where $v_d > v_c$, the real part of χ changes from positive to negative with increasing q , which is consistent with the definition of v_c . To make a further comparison of the degenerate and nondegenerate systems, the q at which the real part of the χ equals zero is plotted as a function of v_d/v_c for both systems in Fig. 5. Both curves are similar for small v_d/v_c , but for very large v_d/v_c , the nondegenerate system has a larger wave-vector range where $\text{Re}[\chi(\omega=0)]$ is positive. We might conclude from this that a drift instability is easier to attain for a nondegenerate system than for a degenerate system at high drift velocities, but these drift ve-

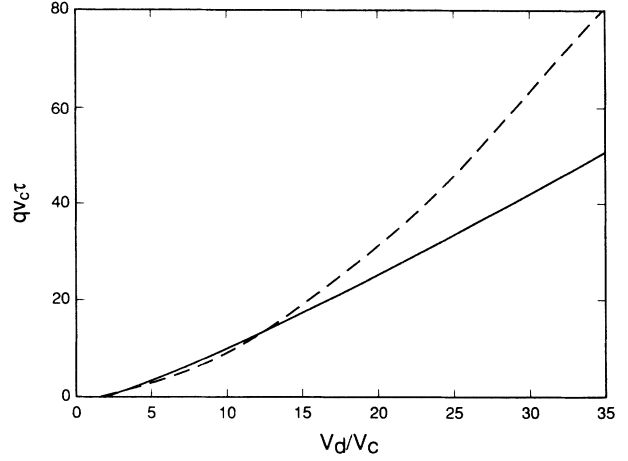


FIG. 5. The wave vector at which the real part of the nonequilibrium static susceptibility $\text{Re}[\chi(q, \omega=0)]$ goes through zero, as a function of the drift velocity, for degenerate (solid lines) and nondegenerate (dashed line) systems, for the classical Boltzmann case ($mv_c^2\tau/\hbar = \infty$). The v_d has to exceed a critical drift velocity v_c (where $v_c = v_{\text{th}}/2$ for nondegenerate systems and $v_c = 1/\sqrt{6}v_F$ for degenerate systems), before $\text{Re}[\chi(\omega=0)]$ exhibits a change in sign from negative to positive with decreasing wave vector. For $v_d < v_c$, $\text{Re}[\chi(\omega=0)]$ is *never* positive for any q . The drift velocities and wave vectors for both curves have been normalized by their respective v_c 's.

locities are so high that they are probably practically unattainable.

V. SUMMARY AND CONCLUSIONS

The method previously applied to a nondegenerate system^{6,7} is used here to calculate the nonequilibrium susceptibility for free carriers in a static electric field in a degenerate system. We extended the Thornber-Price drift-diffusion equation (which includes an electric-field-gradient term) to include effects of degeneracy and used this equation to explain the behavior of the nonequilibrium susceptibilities at small q and ω . For drift velocities above a critical drift velocity v_c (equal to $\frac{1}{2}v_{\text{th}}$ and $(1/\sqrt{6})v_F$ for the nondegenerate and degenerate systems, respectively), the real part of $\chi(q, \omega=0)$ is *positive* for small q . This critical velocity v_c sets a convenient velocity scale for comparisons of the screening of the degenerate and nondegenerate systems. The fact that $\text{Re}[\chi] > 0$ may result, with the proper device configuration, in a system that is unstable to density perturbations under application of a large electric field.

When the nonequilibrium static susceptibilities for the degenerate and nondegenerate systems are scaled by their respective nonequilibrium Lindhard susceptibilities and the drift velocities and wave vectors are scaled by v_c and $v_c\tau$, respectively, the curves of the scaled χ 's for both look remarkably similar. Furthermore, all scaled curves with $mv_c^2\tau/\hbar \gtrsim \max\{1, v_d/v_c\}$ are essentially identical.

One possible extension of this work is to calculate the nonequilibrium susceptibility at arbitrary degeneracy, to

determine if our conjecture that all scaled χ 's independent of degeneracy is in fact correct. Another extension would be to treat cases with more realistic scattering mechanisms to see if the features in the susceptibilities shown in this paper and our previous papers still persist when we go beyond the single-rate relaxation-time approximation. Both Monte Carlo²⁴ and other numerical approaches²⁵ could be used to study screening in nonequilibrium situations.

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APPENDIX A: LINEARIZED SCATTERING OPERATOR

In a nondegenerate system, the scattering operator is

$$S[f_0](\mathbf{p}) = \int d\mathbf{p}' [W(\mathbf{p}; \mathbf{p}') f_0(\mathbf{p}') - W(\mathbf{p}'; \mathbf{p}) f_0(\mathbf{p})], \quad (\text{A1})$$

$$S[f + \delta f] - S[f] \approx S_{\text{lin}}[\delta f]$$

$$= \int d\mathbf{p}' \{ [1 - f_0(\mathbf{p})] W(\mathbf{p}; \mathbf{p}') + W(\mathbf{p}'; \mathbf{p}) f_0(\mathbf{p}) \} \delta f(\mathbf{p}') - \{ [1 - f_0(\mathbf{p}')] W(\mathbf{p}'; \mathbf{p}) + W(\mathbf{p}; \mathbf{p}') f_0(\mathbf{p}') \} \delta f(\mathbf{p}). \quad (\text{A4})$$

Note that S_{lin} is a functional of $f_0(\mathbf{p})$. Physically, $S_{\text{lin}}[\delta f]$ describes the rate of change of a small deviation in the distribution function $\delta f(\mathbf{p})$, due to scattering in the presence of the steady-state distribution function $f_0(\mathbf{p})$.

APPENDIX B: THE DIFFERENTIAL MEAN FREE PATH

In this appendix, we give the formal definition of the differential mean free path $l'(\mathbf{p})$. We also list several properties of $l'(\mathbf{p})$ and give the explicit form of $l'(\mathbf{p})$ for the case of the parabolic band relaxation-time approximation. We begin by introducing the propagator $R(\mathbf{p}', \mathbf{p}; t)$,²⁶ which we use in defining $l'(\mathbf{p})$.

1. The propagator $R(\mathbf{p}', \mathbf{p}; t)$

The quantity $R(\mathbf{p}', \mathbf{p}; t)$ describes the change in the probability of occupation of state \mathbf{p}' at time t , due to the addition of a particle in state \mathbf{p} at $t=0$, in the presence of the steady-state distribution function $f_0(\mathbf{p})$ and the field \mathbf{F}_0 . We show that $R(\mathbf{p}', \mathbf{p}; t)$ satisfies the time-dependent Boltzmann equation with the *linearized* scattering operator.

The evolution of the distribution function, after the addition of a particle in state \mathbf{p} at $t=0$, is given by

$$\left[\frac{\partial}{\partial t} + \mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}'} \right] [f_0(\mathbf{p}') + R(\mathbf{p}', \mathbf{p}; t)] = S[f_0 + R]. \quad (\text{B1})$$

Since $R(\mathbf{p}', \mathbf{p}; t)$ represents an addition of a single parti-

where $W(\mathbf{p}'; \mathbf{p})$ is the scattering rate from state \mathbf{p} to state \mathbf{p}' . This scattering operator is linear in $f_0(\mathbf{p})$, and hence the change in the scattering term due to a change $\delta f(\mathbf{p})$ in the distribution function is

$$S[f_0 + \delta f] - S[f_0] = S[\delta f]. \quad (\text{A2})$$

When a system is degenerate, or when carrier-carrier scattering is present, the scattering operator is nonlinear. For example, in the degenerate case, the scattering operator is

$$S[f_0](\mathbf{p}) = \int d\mathbf{p}' \{ [1 - f_0(\mathbf{p})] W(\mathbf{p}; \mathbf{p}') f_0(\mathbf{p}) - [1 - f_0(\mathbf{p}')] W(\mathbf{p}'; \mathbf{p}) f_0(\mathbf{p}') \}. \quad (\text{A3})$$

However, if the deviation of the distribution function $\delta f(\mathbf{p})$ away from the steady-state distribution function $f_0(\mathbf{p})$ is small, then one can linearize the scattering operator around $f_0(\mathbf{p})$. The change in the scattering term caused by a change $\delta f(\mathbf{p})$ [to linear order in $\delta f(\mathbf{p})$] is given by the linear operator S_{lin}

cle, it is a small perturbation on the distribution function, and therefore the scattering term can be approximated by

$$S[f_0 + R] \approx S[f_0] + S_{\text{lin}}[R]. \quad (\text{B2})$$

Substituting Eq. (B2) into Eq. (B1), and subtracting away the unperturbed Boltzmann equation (i.e., $\mathbf{F}_0 \cdot (\partial f_0 / \partial \mathbf{p}) = S[f_0]$) gives

$$\left[\frac{\partial}{\partial t} + \mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}'} \right] R(\mathbf{p}', \mathbf{p}; t) = \int d\mathbf{p}'' S_{\text{lin}}(\mathbf{p}', \mathbf{p}'') \times R(\mathbf{p}'', \mathbf{p}; t). \quad (\text{B3})$$

Since $R(\mathbf{p}', \mathbf{p}; t)$ represents the insertion of a particle in state \mathbf{p} at $t=0$, the initial condition for $R(\mathbf{p}', \mathbf{p}; t)$ is

$$R(\mathbf{p}', \mathbf{p}; t=0) = \delta(\mathbf{p}' - \mathbf{p}). \quad (\text{B4})$$

When the scattering operator S is linear, $R(\mathbf{p}', \mathbf{p}; t)$ is independent of the distribution $f_0(\mathbf{p})$ of the other particles in the system. $R(\mathbf{p}', \mathbf{p}; t)$ is simply equal to the probability that a particle added at time $t=0$ in state \mathbf{p} is found in the state \mathbf{p}' at time t . However, when the scattering operator is nonlinear, then the *other* particles present in the system affect $R(\mathbf{p}', \mathbf{p}; t)$. For example, if S describes carrier-carrier scattering, then $R(\mathbf{p}', \mathbf{p}; t)$ not only includes the probability that the particle inserted at \mathbf{p} itself scatters into \mathbf{p}' , but also includes the probability that *another* particle in the system scatters into state \mathbf{p}' through an interaction with the inserted particle.

We conclude this section by proving two equalities regarding $R(\mathbf{p}', \mathbf{p}; t)$ which will be useful later. These are

$$R(\mathbf{p}', \mathbf{p}, t = \infty) = \frac{\partial f_0}{\partial n}(\mathbf{p}') \quad (\text{B5})$$

and

$$\int d\mathbf{p} R(\mathbf{p}', \mathbf{p}; t) \frac{\partial f_0}{\partial n}(\mathbf{p}) = \frac{\partial f_0}{\partial n}(\mathbf{p}') \quad \text{for all } t. \quad (\text{B6})$$

To obtain Eq. (B5), we first note that for small uniform change in the density δn , we have

$$\begin{aligned} F_0 \cdot \frac{\partial}{\partial \mathbf{p}} \left[f_0(\mathbf{p}) + \delta n \frac{\partial f_0}{\partial n}(\mathbf{p}) \right] &= S[f_0 + \delta n (\partial f_0 / \partial n)] \\ &\approx S[f_0] + \delta n S_{\text{lin}}[\partial f / \partial n]. \end{aligned} \quad (\text{B7})$$

Subtracting away the unperturbed Boltzmann equation yields

$$F_0 \cdot \frac{\partial f_0}{\partial n}(\mathbf{p}) = S_{\text{lin}}[\partial f_0 / \partial n]. \quad (\text{B8})$$

That is, $\partial f_0 / \partial n$ is the solution of the steady-state Boltzmann equation with the linearized scattering operator S_{lin} . From Eq. (B3), we see that $R(\mathbf{p}', \mathbf{p}; t)$ is the solution of the *time-dependent* Boltzmann equation with S_{lin} . Therefore, as $t \rightarrow \infty$, $R(\mathbf{p}', \mathbf{p}; t)$ approaches the steady-state solution of the linearized Boltzmann equation (assuming that the equation is well-behaved), and therefore $R(\mathbf{p}', \mathbf{p}; t = \infty) = (\partial f_0 / \partial n)(\mathbf{p}')$.

To obtain Eq. (B6), we start by writing the equation for the evolution for $R(\mathbf{p}', \mathbf{p}; t)$ in matrix form

$$\frac{\partial \hat{R}}{\partial t} = \hat{L} \hat{R}, \quad (\text{B9})$$

where

$$L(\mathbf{p}', \mathbf{p}'') = \mathbf{F} \cdot \nabla \delta(\mathbf{p}'' - \mathbf{p}') + S_{\text{lin}}(\mathbf{p}', \mathbf{p}''), \quad (\text{B10})$$

and matrix multiplication means integration over momenta {i.e., $[\hat{L} \hat{R}](\mathbf{p}', \mathbf{p}; t) \equiv \int d\mathbf{p}'' L(\mathbf{p}', \mathbf{p}'') R(\mathbf{p}'', \mathbf{p}; t)$ }. The formal solution for \hat{R} is

$$\hat{R} = \exp(\hat{L}t). \quad (\text{B11})$$

From Eq. (B8), we have

$$\hat{L} \frac{\partial f_0}{\partial n} = 0. \quad (\text{B12})$$

Using Eqs. (B11) and (B12) we obtain

$$\begin{aligned} \hat{R} \frac{\partial f_0}{\partial n} &= \exp(\hat{L}t) \frac{\partial f_0}{\partial n} \\ &= (1 + \hat{L}t + \frac{1}{2} \hat{L}^2 t^2 + \dots) \frac{\partial f_0}{\partial n} \\ &= \frac{\partial f_0}{\partial n}, \end{aligned} \quad (\text{B13})$$

which proves Eq. (B6). Physically, Eq. (B6) simply states that if a small deviation in the distribution function proportional to $(\partial f_0 / \partial n)(\mathbf{p})$ is added at time $t=0$, it remains unchanged for all t .

2. The definition of $l'(\mathbf{p})$

The ‘‘differential mean free path’’ $l'(\mathbf{p})$ is defined by

$$l'(\mathbf{p}) = \int_0^\infty dt \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] R(\mathbf{p}', \mathbf{p}; t), \quad (\text{B14})$$

where $\mathbf{j} = n\mathbf{v}_d$ is the current density and n is the particle density. The derivative $\partial \mathbf{j} / \partial n$ is evaluated at field \mathbf{F}_0 and density n_0 .

When the scattering operator S is linear, $l'(\mathbf{p})$ has a relatively simple interpretation. When S is linear, the drift velocity \mathbf{v}_d is a function of the field \mathbf{F}_0 alone (and not of the density n_0), and hence $\partial \mathbf{j} / \partial n = \mathbf{v}_d$. Furthermore, $R(\mathbf{p}', \mathbf{p}; t)$ is simply equal to the probability that a particle added in the state \mathbf{p} at time $t=0$ propagates to the state \mathbf{p}' in time t . Hence, the average velocity $\overline{\mathbf{v}(t)}$ of an ensemble of particles with initial momentum \mathbf{p} is given by

$$\int d\mathbf{p}' R(\mathbf{p}', \mathbf{p}; t) \mathbf{v}(\mathbf{p}') = \overline{\mathbf{v}(t)}. \quad (\text{B15})$$

Therefore, when the scattering operator is linear, Eq. (B14) is equivalent to

$$l'(\mathbf{p}) = \int_0^\infty dt \overline{\mathbf{v}(t) - \mathbf{v}_d}. \quad (\text{B16})$$

That is, $l'(\mathbf{p})$ is the mean free path of a particle with initial momentum \mathbf{p} in the frame of reference moving with velocity \mathbf{v}_d .

When the scattering operator S is nonlinear, then interpretation of $l'(\mathbf{p})$ is more complex. In this case, $R(\mathbf{p}', \mathbf{p}; t)$ is the probability of occupation of state \mathbf{p}' not only by the particle added in the state \mathbf{p} , but also by other particles that have interacted (directly or indirectly) with the added particle. Therefore, the quantity $\int d\mathbf{p}' R(\mathbf{p}', \mathbf{p}; t) \mathbf{v}(\mathbf{p}')$ is the ensemble average net change of the *sum* of the velocities of *all* the particles in the system, given the addition of a particle in state \mathbf{p} at $t=0$. Hence, when the scattering operator is nonlinear, $l'(\mathbf{p})$ cannot be interpreted as the mean free path of the particle added in state \mathbf{p} .

3. Properties of $l'(\mathbf{p})$

In this section we show that $l'(\mathbf{p})$ satisfies the equation

$$- \left[\mathbf{F} \cdot \frac{\partial}{\partial \mathbf{p}} + S_{\text{lin}}^T \right] l'(\mathbf{p}) = \mathbf{v}(\mathbf{p}) - \frac{\partial \mathbf{j}}{\partial n}, \quad (\text{B17})$$

where S_{lin}^T is the *transpose* of the effective scattering operator, i.e., $S_{\text{lin}}^T(\mathbf{p}, \mathbf{p}') = S_{\text{lin}}(\mathbf{p}', \mathbf{p})$. Physically, S_{lin}^T is the operator that gives the rate of change, due to scattering, of an observable at a given momentum \mathbf{p} , that is,

$$[S_{\text{lin}}^T h](\mathbf{p}) = \left. \frac{dh}{dt}(\mathbf{p}) \right|_{\text{scattering}}. \quad (\text{B18})$$

We also show that

$$\int d\mathbf{p} l'(\mathbf{p}) \frac{\partial f_0}{\partial n}(\mathbf{p}) = 0. \quad (\text{B19})$$

for the case of a single-rate relaxation-time approximation in a parabolic band solid.

a. Proof of Eq. (B17)

These two relations are used in deriving the Thornber-Price drift-diffusion equation. Finally, we evaluate $l'(\mathbf{p})$

To prove Eq. (B17), we substitute the definition of $l'(\mathbf{p})$, Eq. (B14), into the left-hand side of Eq. (B17), which gives

$$-\left[\mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} + S_{\text{lin}}^T \right] l'(\mathbf{p}) = - \int_0^\infty dt \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] \left[\mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} R(\mathbf{p}', \mathbf{p}; t) + \int d\mathbf{p}'' S_{\text{lin}}(\mathbf{p}, \mathbf{p}'') R(\mathbf{p}', \mathbf{p}''; t) \right]. \quad (\text{B20})$$

We show below that the right-hand side of Eq. (B20) is equal to $\mathbf{v}(\mathbf{p}) - \partial \mathbf{j} / \partial n$.

The term in the second set of large parentheses on the right-hand side of Eq. (B20) can be written in matrix form, with \hat{L} defined in Eq. (B10):

$$\begin{aligned} \mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} R(\mathbf{p}', \mathbf{p}; t) + \int d\mathbf{p}'' S_{\text{lin}}^T(\mathbf{p}, \mathbf{p}'') R(\mathbf{p}', \mathbf{p}''; t) &= \int d\mathbf{p}'' R(\mathbf{p}', \mathbf{p}'') [\mathbf{F}_0 \cdot \nabla \delta(\mathbf{p} - \mathbf{p}'') + S_{\text{lin}}(\mathbf{p}'', \mathbf{p})] \\ &\equiv \hat{R} \hat{L} = \hat{L} \hat{R} = \frac{\partial \hat{R}}{\partial t}. \end{aligned} \quad (\text{B21})$$

The penultimate equality in Eq. (B21), that \hat{L} commutes with \hat{R} , is due to Eq. (B11). The last equality in Eq. (B21) is Eq. (B9).

Substituting Eq. (B21) into Eq. (B20) yields

$$\begin{aligned} - \left[\mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} + S_{\text{lin}}^T \right] l'(\mathbf{p}) &= - \int d\mathbf{p}' \int_0^\infty dt \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] \frac{\partial \hat{R}}{\partial t} \\ &= - \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] [R(\mathbf{p}', \mathbf{p}; t = \infty) - R(\mathbf{p}', \mathbf{p}; t = 0)]. \end{aligned} \quad (\text{B22})$$

The term corresponding to $R(\mathbf{p}', \mathbf{p}; t = \infty)$ in Eq. (B22) gives zero contribution because from Eq. (B5)

$$\begin{aligned} \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] R(\mathbf{p}', \mathbf{p}; t = \infty) &= \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] \frac{\partial f_0}{\partial n}(\mathbf{p}') \\ &= \int \frac{\partial}{\partial n} \left[\int d\mathbf{p}' \mathbf{v}(\mathbf{p}') f_0(\mathbf{p}') \right] - \frac{\partial \mathbf{j}}{\partial n} \\ &= \left[\frac{\partial \mathbf{j}}{\partial n} - \frac{\partial \mathbf{j}}{\partial n} \right] = 0. \end{aligned} \quad (\text{B23})$$

Hence, using Eq. (B23) and the initial condition for $R(\mathbf{p}', \mathbf{p}; t)$, Eq. (B4), we obtain from Eq. (B22)

$$-\left[\mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} + S_{\text{lin}}^T \right] l'(\mathbf{p}) = \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] \delta(\mathbf{p}' - \mathbf{p}) = \mathbf{v}(\mathbf{p}) - \frac{\partial \mathbf{j}}{\partial n}. \quad (\text{B24})$$

This proves Eq. (B17).

b. Proof of Eq. (B19)

To prove Eq. (B19), we multiply both sides of Eq. (B14) by $(\partial f_0 / \partial n)(\mathbf{p})$ and integrate over \mathbf{p} , giving

$$\int d\mathbf{p} l'(\mathbf{p}) \frac{\partial f_0}{\partial n}(\mathbf{p}) = \int_0^\infty dt \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] \left[\int d\mathbf{p} R(\mathbf{p}', \mathbf{p}; t) \frac{\partial f_0}{\partial n}(\mathbf{p}) \right]. \quad (\text{B25})$$

Substituting Eq. (B6) into the right-hand side of Eq. (B25) gives

$$\begin{aligned} \int d\mathbf{p} l'(\mathbf{p}) \frac{\partial f_0}{\partial n}(\mathbf{p}) &= \int_0^\infty dt \int d\mathbf{p}' \left[\mathbf{v}(\mathbf{p}') - \frac{\partial \mathbf{j}}{\partial n} \right] \frac{\partial f_0}{\partial n}(\mathbf{p}') \\ &= \int_0^\infty dt \left[\frac{\partial}{\partial n} \left[\int d\mathbf{p}' \mathbf{v}(\mathbf{p}') f_0(\mathbf{p}') \right] \right. \\ &\quad \left. - \frac{\partial \mathbf{j}}{\partial n} \right] \\ &= \int_0^\infty dt \left[\frac{\partial \mathbf{j}}{\partial n} - \frac{\partial \mathbf{j}}{\partial n} \right] = 0, \end{aligned} \quad (\text{B26})$$

which is the desired result.

c. Evaluation of $l'(\mathbf{p})$ for the single-rate relaxation-time approximation in a parabolic band

We show that, within this approximation,

$$l'(\mathbf{p}) = \frac{1}{m} (\mathbf{p} - \mathbf{F}_0 \tau) \tau = (\mathbf{v} - \mathbf{v}_d) \tau. \quad (\text{B27})$$

The scattering operator within this approximation is

$$S[f] = - \frac{f(\mathbf{p}) - f_{\text{eq}}(\mathbf{p}, n)}{\tau}, \quad (\text{B28})$$

where the density of the equilibrium distribution function is given by conservation of particles

$$\int d\mathbf{p} f_{\text{eq}}(\mathbf{p}, n) = \int d\mathbf{p} f(\mathbf{p}). \quad (\text{B29})$$

The linearized scattering operator is given by

$$S_{\text{lin}}[\delta f] = - \frac{\delta f(\mathbf{p}) - \delta n (\partial f_{\text{eq}} / \partial n)(\mathbf{p})}{\tau}, \quad (\text{B30})$$

where $\delta n = \int d\mathbf{p} \delta f(\mathbf{p})$. From Eq. (B30), we obtain the matrix form of S_{lin} ,

$$S_{\text{lin}}(\mathbf{p}, \mathbf{p}') = - \frac{1}{\tau} \left[\delta(\mathbf{p}' - \mathbf{p}) - \frac{\partial f_{\text{eq}}}{\partial n}(\mathbf{p}) \right]. \quad (\text{B31})$$

[Recall that matrix multiplication is defined by $S_{\text{lin}} f(\mathbf{p}) = \int d\mathbf{p}' S_{\text{lin}}(\mathbf{p}, \mathbf{p}') f(\mathbf{p}')$.] Hence, from Eq. (B31), the transpose of S_{lin} is

$$S_{\text{lin}}^T(\mathbf{p}, \mathbf{p}') = - \frac{1}{\tau} \left[\delta(\mathbf{p}' - \mathbf{p}) - \frac{\partial f_{\text{eq}}}{\partial n}(\mathbf{p}') \right]. \quad (\text{B32})$$

On substituting Eq. (B32) into Eq. (B17) (the integrodifferential equation that $l'(\mathbf{p})$ satisfies) and using the fact that in the single-rate relaxation-time approximation in a parabolic band, $\mathbf{v} = \mathbf{p}/m$ and $\partial \mathbf{j} / \partial n = \mathbf{F}_0 \tau / m = \mathbf{v}_d$, we obtain

$$\begin{aligned} -\mathbf{F}_0 \cdot \frac{\partial l'}{\partial \mathbf{p}} - \frac{1}{\tau} \int d\mathbf{p}' \frac{\partial f_{\text{eq}}}{\partial n}(\mathbf{p}') l'(\mathbf{p}') + \frac{1}{\tau} l'(\mathbf{p}) \\ = \frac{1}{m} (\mathbf{p} - \mathbf{F}_0 \tau). \end{aligned} \quad (\text{B33})$$

Equation (B33) is the equation that determines l' , up to an additive constant, in the parabolic-band single-rate

relaxation-time approximation. The additive constant is determined by Eq. (B19). Equations (B33) and (B19) show that Eq. (B27) is the correct expression, within this approximation, for $l'(\mathbf{p})$. One can easily verify this by substituting the expression for $l'(\mathbf{p})$ from Eq. (B27) into Eqs. (B33) and (B19). Both substitutions give the correct result.

**APPENDIX C:
DETAILS OF THE DERIVATION
OF THE THORNBUR-PRICE
DRIFT-DIFFUSION EQUATION**

In this appendix, we provide some of the details of the derivation of Thornber and Price's extension of the conventional drift-diffusion equation.^{9,10} We also further extend it to include (1) a *nonlinear* scattering term in the transport equation and (2) temporal variations. We refer to this equation (with the extensions for nonlinear scattering and temporal variations) as the Thornber-Price drift-diffusion equation. We start from the Boltzmann equation.

The Boltzmann equation is

$$\frac{1}{n} \frac{\partial (ng)}{\partial t} + \mathbf{F} \cdot \frac{\partial g}{\partial \mathbf{p}} + \frac{1}{n} \mathbf{v} \cdot \nabla (ng) = \frac{1}{n} S[ng], \quad (\text{C1})$$

where $g(\mathbf{p}, \mathbf{x}, t) = f(\mathbf{p}, \mathbf{x}, t) / n(\mathbf{x}, t)$, so that $\int g(\mathbf{p}, \mathbf{x}, t) d\mathbf{p} = 1$. The unperturbed Boltzmann equation then reads

$$\mathbf{F}_0 \cdot \frac{\partial g_0}{\partial \mathbf{p}} = \frac{1}{n_0} S[n_0 g_0], \quad (\text{C2})$$

where the subscripts "0" refers to the steady-state homogeneous electric field quantities. Then, we assume small perturbations about the steady homogeneous state

$$\begin{aligned} g(\mathbf{p}, \mathbf{x}, t) &= g_0(\mathbf{p}) + \delta g(\mathbf{p}, \mathbf{x}, t), \\ n(\mathbf{p}, \mathbf{x}, t) &= n_0 + \delta n(\mathbf{x}, t), \\ \mathbf{F}(\mathbf{x}, t) &= \mathbf{F}_0 + \delta \mathbf{F}(\mathbf{x}, t), \\ S[f_0 + \delta f] &= S[f_0] + S_{\text{lin}}[\delta f], \\ \delta f(\mathbf{p}, \mathbf{x}, t) &= n_0 \delta g(\mathbf{p}, \mathbf{x}, t) + \delta n(\mathbf{x}, t) g_0(\mathbf{p}). \end{aligned} \quad (\text{C3})$$

Substituting Eqs. (C3) into the Boltzmann equation, Eq. (C1), and subtracting the unperturbed Boltzmann equation, Eq. (C2), gives

$$\begin{aligned} \left[S_{\text{lin}} - \mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} \right] \delta g &= \delta \mathbf{F} \cdot \frac{\partial g_0}{\partial \mathbf{p}} + \frac{1}{n_0} g_0 \mathbf{v} \cdot \nabla n \\ &\quad + \mathbf{v} \cdot \nabla \delta g + \frac{g_0}{n_0} \frac{\partial \delta n}{\partial t} \\ &\quad + \frac{\partial \delta g}{\partial t} - \frac{\delta n}{n_0} S_{\text{lin}} g_0. \end{aligned} \quad (\text{C4})$$

Multiplying the left-hand side of Eq. (C4) by $l'(\mathbf{p})$ and integrating over \mathbf{p} gives

$$\int d\mathbf{p} l'(\mathbf{p}) \left[S_{\text{lin}} - \mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} \right] \delta g(\mathbf{p}) = \int d\mathbf{p} \delta g(\mathbf{p}) \left[S_{\text{lin}}^T + \mathbf{F}_0 \cdot \frac{\partial}{\partial \mathbf{p}} \right] l'(\mathbf{p})$$

$$= -\delta \mathbf{u}, \quad (\text{C5})$$

where we have used Eq. (B17) to obtain the last equality in Eq. (C5). By multiplying both sides of Eq. (C4) by $l'(\mathbf{p})$ and integrating over \mathbf{p} we obtain, using Eq. (C5)

$$-\delta \mathbf{u}(\mathbf{x}, t) = \int d\mathbf{p} l'(\mathbf{p}) \delta \mathbf{F}(\mathbf{x}, t) \frac{\partial g_0}{\partial \mathbf{p}} + \frac{\nabla n(\mathbf{x}, t)}{n_0} \cdot \int d\mathbf{p} g_0(\mathbf{p}) \mathbf{v}(\mathbf{p}) l'(\mathbf{p})$$

$$+ \int d\mathbf{p} l'(\mathbf{p}) \mathbf{v} \cdot \nabla g(\mathbf{p}, \mathbf{x}, t) + \frac{1}{n_0} \frac{\partial n(\mathbf{x}, t)}{\partial t} \int d\mathbf{p} l'(\mathbf{p}) g_0(\mathbf{p}) + \int d\mathbf{p} l'(\mathbf{p}) \frac{\partial g(\mathbf{p}, \mathbf{x}, t)}{\partial t}$$

$$- \frac{\delta n}{n_0} \int d\mathbf{p} S_{\text{lin}}[g_0](\mathbf{p}) l'(\mathbf{p}). \quad (\text{C6})$$

After integrating the $\delta \mathbf{F}$ terms by parts, we obtain Eq. (3.5). This equation is *exact* to linear order in the perturbations. Unfortunately, it requires the knowledge of the linear-order change in the distribution function $\delta g(\mathbf{p}, \mathbf{x}, t)$, which can only be obtained from solving the transport equation. In the text, this equation is used in conjunction with the approximation that assumes $\delta g(\mathbf{p}, \mathbf{x}, t)$ is only dependent on the local electric field and density, to obtain a drift-diffusion type of equation with $\nabla \mathbf{F}$, $\partial \mathbf{F} / \partial t$ and δn correction terms, which we refer to as the Thornber-Price drift-diffusion equation.

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