

Anisotropic scattering in quantum magnetotransport calculations for two-dimensional electron systems in a one-dimensional superlattice

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Based on the self-consistent Born approximation for the evaluation of Kubo formulas, we develop and evaluate a consistent approximation scheme that allows us to calculate the magnetoconductivity tensor for a high-mobility two-dimensional electron system, subjected to a weak periodic potential modulation in one lateral direction, under due consideration of anisotropic impurity scattering. We demonstrate that our approach avoids the inconsistencies observed with previous calculations based on a c -number approximation for the self-energy operator, and that it is able to reproduce, with reasonable assumptions for the finite-range impurity potentials, nearly quantitatively the experimental results for all components of the magnetoresistance tensor in the regime of moderate and strong magnetic fields, which are characterized by commensurability and Shubnikov–de Haas oscillations, respectively.

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I. INTRODUCTION

The importance of anisotropic scattering for a quantitative understanding of magnetotransport experiments in modulated two-dimensional electron systems (2DES's) was recently emphasized in classical magnetotransport calculations.^{1,2} To include this anisotropy, one has to go conceptually beyond the assumption of a constant (i.e., energy- and magnetic-field independent) transport relaxation time, that had been the basis of early quantum³ and classical⁴ calculations, which could explain the observed commensurability oscillations qualitatively. However, because of the numerical difficulties, quantum calculations including anisotropic impurity scattering within the framework of the self-consistent Born approximation (SCBA) were attempted only recently,⁵ whereas most approaches used the so-called c -number approximation (CNA),^{6,7} which was introduced by Zhang and Gerhardt.⁶ Unfortunately, this approximation, which neglects vertex corrections to the transport coefficients, is questionable since it violates the continuity equation for the modulated system, as is known from the corresponding classical relaxation time approximation.¹ Furthermore, it can describe only isotropic scattering, leading to a coarse, unsatisfactory picture of the experimental data. On the other hand, the CNA allows an intuitive understanding of the experiment in terms of a band and a scattering conductivity,⁶ which is appropriate for small and moderate values of the magnetic field B , where, at least for short-range impurity scattering, the vertex corrections are relatively small.¹

To overcome the problems with the CNA, one can try to solve the full SCBA. Because of the complexity of the required numerics, this has been possible only for a very limited and unrealistic parameter range.⁵ On the other hand, due to the complicated nature of the self-consistent Dyson and Bethe-Salpeter equations, which govern the equilibrium and the transport regime, respectively, the results are hard to interpret. We, therefore, do not try to solve the full SCBA, but improve the CNA to achieve a consistent approximation

which describes correctly the impurity-scattering processes in the 2DES. Our approximation scheme assumes a weak potential modulation and a high mobility, i.e., small collision broadening of the Landau levels. In contrast to previous work,^{6,5} we present also a careful consistent treatment of the Hall conductivity σ_H , which allows us to relate the different appearances of σ_H -versus- B traces measured on Si-MOSFET's and on (AlGa)As heterostructures to the different properties of the relevant impurity-scattering in both materials. Some preliminary results of our approach have already been published elsewhere.⁸

The paper is organized as follows. In Sec. II we briefly recall the basic results of the (Kubo-type) linear response theory within the SCBA as applied to magnetotransport in a laterally modulated 2DES. In Sec. III we formulate our basic approximation and exploit its consequences for the conductivity tensor. Typical results of our numerical calculations are presented in Sec. IV A, and an explicit comparison with experiment is given in Sec. IV B. In Appendix A we sketch the derivation of the SCBA kernel (Appendix A1), exploit the Ward identities for the calculation of the SCBA conductivities (Appendix A2) and show that the quantum correction to the Hall conductivity is a Fermi edge quantity (Appendix A3). In Appendix B we specify these results to our weak-modulation approximation.

II. THEORETICAL FRAMEWORK

Our aim is to extend the approach of Ref. 9, which treats homogeneous systems, to the case of a noninteracting 2DES in a weak modulation potential, e.g., $V(x) = V_0 \cos Kx$, with period $a = 2\pi/K$. We will take into account the modulation effects to lowest order in the small parameter $V_0/\hbar\omega_0$, where $\omega_0 = eB_0/m$ is the cyclotron frequency in the applied perpendicular magnetic field B_0 . But before we enter the corresponding perturbation expansion, we briefly recall the underlying Kubo-type magnetotransport theory.

A. Green and vertex operators

We describe the “clean” system without impurities by the Hamiltonian

$$H = (m/2)\mathbf{v}^2 + V(x), \quad \mathbf{v} = [\mathbf{p} + e\mathbf{A}(x)]/m, \quad (1)$$

with the vector potential $\mathbf{A}(x) = (0, xB_0)$, so that the Hamiltonian has translational invariance in y direction and p_y is a constant of motion. To describe the effect of random impurity scattering, we first introduce a random configuration of impurities defining the potential energy $V_i(\mathbf{r})$ for a conduction electron, and express equilibrium and transport quantities in terms of the Green operator $\mathcal{G}^\pm(E) = (E - H - V_i \pm i0)^{-1}$. Using conventional perturbation expansion with respect to V_i , we carry out the average over all possible impurity configurations term by term and resum the perturbation series to obtain Dyson's equation for the averaged Green function and the Bethe-Salpeter equation for the transport quantities.

The effect of random impurity scattering on equilibrium quantities is given by the averaged Green operator

$$G^\pm(E) = \langle \mathcal{G}^\pm(E) \rangle = [E - H - \Sigma^\pm(E)]^{-1}, \quad (2)$$

which usually is expressed in terms of the self-energy operator $\Sigma^\pm(E)$. The components of the static conductivity tensor are calculated from the vertex operators

$$F_v^{\sigma\sigma'}(E, E') = \langle \mathcal{G}^\sigma(E) v_\nu \mathcal{G}^{\sigma'}(E') \rangle, \quad (3)$$

with $\sigma, \sigma' \in \{+, -\}$, according to⁹

$$\sigma_{\mu\nu} = \frac{e^2 \hbar}{4\pi S} \int dE \left[\frac{-df}{dE} \phi_{\mu\nu}^{(1)}(E) + f(E) \phi_{\mu\nu}^{(2)}(E) \right], \quad (4)$$

$$\phi_{\mu\nu}^{(1)}(E) = \text{Tr } v_\mu (2F_\nu^{+-} - F_\nu^{++} - F_\nu^{--}), \quad (5)$$

$$\phi_{\mu\nu}^{(2)}(E) = \text{Tr } v_\mu (D_\nu^- - D_\nu^+), \quad (6)$$

where $\nu, \mu \in \{x, y\}$, $v_\mu = (p_\mu + eA_\mu)/m$ is a component of the velocity operator, S the area of the 2DES, and $f(E)$ the Fermi function. Here we use the notation

$$F_v^{\sigma\sigma'} = F_v^{\sigma\sigma'}(E, E), \quad (7)$$

$$D_\nu^\sigma = (\partial/\partial E - \partial/\partial E') F_\nu^{\sigma\sigma}(E, E')|_{E=E'}. \quad (8)$$

It can be shown easily (cyclic invariance of the trace) that the diagonal terms $\phi_{\mu\mu}^{(2)}(E)$ vanish, so that contributions to the diagonal components of the conductivity come only from the Fermi edge

$$\sigma_{\mu\mu} = \int_{-\infty}^{\infty} dE \left[-\frac{df}{dE} \right] \sigma_{\mu\mu}(E). \quad (9)$$

In evaluating the impurity-averaged Green and vertex operators, certain consistency relations (“Ward identities”) have to be obeyed, which can be derived from the equation of continuity.¹⁰ The simplest of these reads

$$F_v^{\sigma\sigma} = \frac{i}{\hbar} [G^\sigma(E), r_\nu], \quad (10)$$

where r_ν is a component of the position operator, $i[H, r_\nu] = \hbar v_\nu$, and follows from $[G^\sigma, r_\nu] = \mathcal{G}^\sigma[H, r_\nu] \mathcal{G}^\sigma = -i\hbar \mathcal{G}^\sigma v_\nu \mathcal{G}^\sigma$.

B. SCBA

We evaluate impurity averages within the self-consistent Born approximation (SCBA), the simplest approximation scheme that allows to satisfy the Ward identities. For simplicity we assume a potential landscape $V_i(\mathbf{r}) = \sum_j u(\mathbf{r} - \mathbf{R}_j)$ of only one type of impurities $u(\mathbf{r})$ located at positions \mathbf{R}_j . Then the SCBA expression for the self-energy is

$$\Sigma^\pm(E) = I[G^\pm(E)], \quad (11)$$

$$I[O] = n_i \int d\mathbf{R} u(\mathbf{r} - \mathbf{R}) O u(\mathbf{r} - \mathbf{R}), \quad (12)$$

with n_i the impurity density and O an arbitrary operator. Thus Eq. (2) becomes the nonlinear Dyson equation from which self-energy and Green operator must be calculated. If these are known, one has to calculate the vertex operators from the linear Bethe-Salpeter equations

$$F_v^{\sigma\sigma'} = G^\sigma(E) \{v_\nu + I[F_v^{\sigma\sigma'}]\} G^{\sigma'}(E'), \quad (13)$$

where the energy arguments of $F_v^{\sigma\sigma'}(E, E')$ are suppressed. The vertex corrections $I[F_v^{\sigma\sigma'}]$ do in general not vanish, and the vertex operator F_v^{+-} can in general not be expressed in terms of the Green operators $G^\pm(E)$. With Eqs. (2) and (13), the Ward identities (10) read

$$[\Sigma^\sigma, r_\nu] = I[[G^\sigma, r_\nu]]. \quad (14)$$

1. Landau representation

As a convenient basis for numerical calculations, we choose the Landau basis $|n, X\rangle$ of eigenstates of the homogeneous system, where n counts the Landau levels with energies $\epsilon_n = \hbar \omega_0(n + 1/2)$ and the “center coordinate” $X = -p_y/(m\omega_0)$ is given by the eigenvalues p_y of the canonical momentum. The conservation of this momentum is an immediate consequence of the translation invariance in y direction and holds also for the impurity averaged and in x direction modulated systems to be considered in the following.

Due to the translation invariance in y direction, both Green function and self-energy must have Landau matrix elements of the form $\langle n, X | G^\pm(E) | n', X' \rangle = \delta_{X', X} G_{n, n'}^\pm(E; X)$. Since the energy eigenvalues of the Hamiltonian (1), $E_n(X) = E_n(X + a)$, are periodic,¹¹ one can employ methods as in Ref. 9 to show that also the matrix elements $G_{n, n'}^\pm(E; X)$ and the corresponding matrix elements of self-energy and vertex operators are periodic in X with the period a of the modulation in x direction. Using Fourier expansions of $\Sigma_{n, n'}^\pm(E; X)$ and $G_{n, n'}^\pm(E; X)$, we show in Appendix A1 that Eq. (11) can be written in the convolution form

$$\Sigma_{n, m}^\pm(E; X) = \sum_{k, l} \int_0^a \frac{dX'}{a} K_{k, l}^{n, m}(X - X') G_{k, l}^\pm(E; X'), \quad (15)$$

where the kernel obtained from the SCBA definition (12) is also periodic with respect to its argument. It has the Fourier expansion and the symmetry properties

$$K_{k,l}^{n,m}(X) = \sum_{\lambda} K_{k,l}^{\lambda;n,m} e^{i\lambda KX} = K_{l,k}^{m,n}(X) = K_{n,m}^{k,l}(-X). \quad (16)$$

This kernel also determines the vertex corrections, i.e., the integral operator, in the Bethe-Salpeter equation (13).

2. Conductivities in SCBA

Due to the Ward identities (10) there is no need to solve the Bethe-Salpeter equations for $F_v^{\sigma\sigma}$. However, one has to evaluate the Ward identities with some care, since the contributions of the $F_v^{\sigma\sigma}$ to the diagonal components of the conductivity tensor diverge and must cancel corresponding contributions to F_v^{+-} .⁹ The evaluation is easiest for σ_{xx} . Since $G^{\sigma}(E)$ is diagonal in the center coordinate X and, according to Eq. (1), the operator identity

$$r_x \equiv x = X + v_y / \omega_0 \quad (17)$$

holds, we obtain from Eq. (10)

$$F_x^{\sigma\sigma} = \frac{i}{\hbar \omega_0} [G^{\sigma}(E), v_y]. \quad (18)$$

Following Ref. 9, we make the ansatz [suppressing the energy arguments]

$$F_x^{+-} = \tilde{F}_x^{+-} + \frac{i}{\hbar \omega_0} (G^+ v_y - v_y G^-) \quad (19)$$

and obtain

$$\sigma_{xx}(E) = \frac{e^2 \hbar}{2\pi S} \text{Tr} \left[v_x \tilde{F}_x^{+-} + \frac{\pi}{\hbar \omega_0} \{v_x, v_y\} A \right], \quad (20)$$

with the notations $\{v_x, v_y\} = v_x v_y + v_y v_x$ for the anticommutator and $A(E) = [G^-(E) - G^+(E)] / (2\pi i)$ for the spectral operator. Inserting the ansatz (19) into Eq. (13), we obtain the integral equation

$$\tilde{F}_x^{+-} = G^+ (-C[v_y] / \omega_0 + I[\tilde{F}_x^{+-}]) G^-, \quad (21)$$

where the inhomogeneous term is now given in terms of the ‘‘generalized collision operator’’⁹

$$C[\phi] = \frac{i}{\hbar} (\Sigma^+ \phi - \phi \Sigma^- - I[G^+ \phi - \phi G^-]). \quad (22)$$

With the notation $\Sigma^- - \Sigma^+ = i\Gamma$, this collision operator is the sum of two terms $C = C_1 + C_2$, the first of which

$$C_1[\phi] = \frac{1}{2\hbar} (\Gamma \phi + \phi \Gamma) - \frac{\pi}{\hbar} I[A \phi + \phi A], \quad (23)$$

resembles the collision operator of the Boltzmann equation and reduces in the simplest approximation to a relaxation rate,⁹ while the second

$$C_2[\phi] = \frac{i}{2\hbar} (I[\Sigma^- + \Sigma^+, \phi] - I[[G^- + G^+, \phi]]), \quad (24)$$

has a commutator structure. The solution $\tilde{F}_x^{+-}(E)$ of Eq. (21) completely determines σ_{xx} .

To evaluate the contribution of the Ward identities to σ_{yy} we cannot use the same type of arguments, as we demonstrate in Appendix A2. Nevertheless, we can derive

$$\text{Tr } v_y F_y^{\sigma\sigma} = \text{Tr } v_y \left[-\frac{i}{\hbar \omega_0} [G^{\sigma}(E), v_x] \right] \quad (25)$$

as a weaker analog of Eq. (18). Then with the ansatz

$$F_y^{+-} = \tilde{F}_y^{+-} - \frac{i}{\hbar \omega_0} (G^+ v_x - v_x G^-), \quad (26)$$

similar to Eq. (19), we get

$$\sigma_{yy}(E) = \frac{e^2 \hbar}{2\pi S} \text{Tr} \left[v_y \tilde{F}_y^{+-} - \frac{\pi}{\hbar \omega_0} \{v_x, v_y\} A \right]. \quad (27)$$

Introducing Eq. (26) into Eq. (13) and exploiting the equation $[v_x, H] = -i\hbar \omega_0 v_y - i(\hbar/m) dV(x)/dx$ [see Eq. (1)], we now obtain

$$\tilde{F}_y^{+-} = G^+ \left(\frac{C[v_x]}{\omega_0} - \frac{1}{m\omega_0} \frac{dV}{dx} + I[\tilde{F}_x^{+-}] \right) G^-, \quad (28)$$

where the explicit appearance of the modulation potential destroys the symmetry between Eqs. (21) and (28).

We can further show (Appendix A3) that the off-diagonal components of the conductivity tensor can be written as

$$\sigma_{\mu\nu} = \sigma_{\mu\nu}^{(0)} + \int dE \left[-\frac{df}{dE} \right] \sigma_{\mu\nu}^{\text{sc}}(E), \quad (29)$$

where

$$\sigma_{yx}^{(0)} = -\sigma_{xy}^{(0)} = e^2 n_{\text{el}} / (m\omega_0) \quad (30)$$

is the Hall conductivity of a homogenous 2DES of density n_{el} in the absence of impurity scattering. The contribution due to impurity scattering effects can be written (see Appendix A3)

$$\sigma_{xy}^{\text{sc}}(E) = \frac{e^2 \hbar}{4\pi S} \text{Tr} \left(2v_x \tilde{F}_y^{+-} - \frac{4\pi}{\hbar \omega_0} (v_x^2 - v_y^2) A(E) - \frac{\partial(G^- + G^+)}{\partial p_y} \frac{C_1[v_y]}{\omega_0} \right) \quad (31)$$

and

$$\sigma_{yx}^{\text{sc}}(E) = \frac{e^2 \hbar}{4\pi S} \text{Tr} \left(2v_y \tilde{F}_x^{+-} + \frac{\partial(G^- + G^+)}{\partial p_y} \frac{C_1[v_y]}{\omega_0} \right). \quad (32)$$

Note that, in addition to the second term on the right-hand side of Eq. (31), there is an asymmetry in the integral equations (28) and (21) defining \tilde{F}_y^{+-} and \tilde{F}_x^{+-} , respectively. We will not further investigate the relation between $\sigma_{yx}^{\text{sc}}(E)$ and $\sigma_{xy}^{\text{sc}}(E)$ in the general SCBA, since we will introduce an additional approximation for the numerical calculations that will yield $\sigma_{xy}^{\text{sc}}(E) = -\sigma_{yx}^{\text{sc}}(E)$.

3. Homogeneous 2DES

In the homogeneous system the Green operator $G_{n,m}^{\pm}(E;X) = \delta_{n,m} G_n^{\pm}(E)$ is diagonal in the Landau basis, provided the impurity potentials have rotational symmetry, and the matrix elements of both G and the vertex operators $F_{\mu}^{\sigma\sigma'}$ are independent of X .^{9,10} As a consequence, the SCBA kernel (16) reduces to

$$K_{k,l}^{n,m}(X) = K_{k,l}^{\lambda=0;n,m} \propto \delta_{n-m,k-l}, \quad (33)$$

see Eq. (A3). Owing to these selection rules, Eq. (15) reduces to

$$\Sigma_n^{\pm}(E) = \sum_k K_{k,k}^{0;n,n} G_k^{\pm}(E), \quad (34)$$

i.e., the self-energy becomes diagonal and independent of X , and the matrix elements of the vertex operators in the Landau representation have the same structure as the velocity operators

$$\begin{aligned} \langle n,X|v_{\pm}|m,X\rangle &\equiv \langle n,X|(v_x \pm iv_y)|m,X\rangle \\ &= \pm il_0 \omega_0 \sqrt{2m+1 \pm 1} \delta_{n,m \pm 1}, \end{aligned} \quad (35)$$

where $l_0 = \sqrt{\hbar/(m\omega_0)}$ is the magnetic length. These matrix elements are purely off-diagonal with respect to the Landau quantum numbers n and m , with nonzero values only between adjacent Landau levels. This simple matrix structure simplifies the solution of the Bethe-Salpeter equation considerably. Since the anticommutator $\{v_x, v_y\} = (v_+^2 - v_-^2)/(2i)$ and the difference $v_x^2 - v_y^2 = (v_+^2 + v_-^2)/2$ have no diagonal Landau matrix elements, the corresponding terms in Eqs. (20), (27), and (31) vanish. The x and y directions are now physically equivalent, and one obtains

$$\sigma_{xx}^{\text{hom}}(E) = \sigma_{yy}^{\text{hom}}(E) = \frac{e^2 \hbar}{2\pi S} \text{Tr } v_x \tilde{F}_x^{+-}(E). \quad (36)$$

One can also show that the homogeneous system obeys in the SCBA⁹

$$\sigma_{yx}^{\text{sc}}(E) = -\sigma_{xy}^{\text{sc}}(E) = \frac{e^2 \hbar}{2\pi S} \text{Tr} \frac{C[v_x]}{\omega_0} \tilde{F}_x^{+-}(E). \quad (37)$$

For isotropic scattering, i.e., δ -potential impurities, Σ becomes also independent of the Landau quantum number n , which leads to

$$\Sigma^{\pm}(E) = \frac{n_i \mu_0}{2\pi l_0^2} \sum_k G_k^{\pm}(E), \quad (38)$$

where a high-energy cutoff needs to be introduced to make the sum convergent. In this case the vertex corrections vanish and Eq. (13) reduces to $F_{\nu}^{\sigma\sigma'}(E, E') = G^{\sigma}(E) v_{\nu} G^{\sigma'}(E)$. The relation between Hall and diagonal conductivity, Eq. (37), simplifies in this case to

$$\sigma_{yx}^{\text{sc}}(E) = -\sigma_{xy}^{\text{sc}}(E) = \frac{\Gamma(E)}{\hbar \omega_0} \sigma_{xx}^{\text{hom}}(E). \quad (39)$$

All this is no longer true for anisotropic scattering, and, in general, also not for periodically modulated systems, even if the scattering potentials are δ -function-like. Moreover, in general, there is no shared eigensystem of H , G , and Σ .

III. H-DIAGONAL APPROXIMATION (HDA)

A. Motivation

Compared with the homogeneous Landau system, the modulation potential $V(x)$ introduces as a qualitatively new phenomenon current carrying energy eigenstates $|n, X\rangle$, $H|n, X\rangle = E_n(X)|n, X\rangle$, with a finite group velocity in the y direction

$$\langle n, X|v_y|n, X\rangle = -\frac{1}{m\omega_0} \frac{dE_n(X)}{dX}, \quad (40)$$

while $\langle n, X|v_x|n, X\rangle = 0$ still holds, as in the unmodulated system. [We denote the eigenstates of the modulated system by $|n, X\rangle$ to distinguish them from the Landau states $|n, X\rangle$, with $\langle n, X|v_{\mu}|n, X\rangle = 0$ for $\mu = x$ and $\mu = y$.] In high-mobility systems, this unbounded motion in energy eigenstates leads to a ‘‘band conductivity’’ contribution⁶ to σ_{yy} that increases with decreasing impurity-scattering rate (just as the conductivity in the absence of a magnetic field), whereas the usual diffusive magnetoconductivity (‘‘scattering conductivity’’) is nonzero only because of impurity scattering and decreases with decreasing scattering rate.⁸ For a rough estimate, we may neglect vertex corrections to obtain

$$\sigma_{yy}(E) \sim \frac{\pi e^2 \hbar}{S} \text{Tr } v_y A(E) v_y A(E). \quad (41)$$

Furthermore, we may assume that the spectral operator is dominated by its diagonal elements, which we estimate as $A_n(E; X) \approx (\Gamma_n/2\pi)/[(E - E_n)^2 + (\Gamma_n/2)^2]$ with $|E_n - \hbar\omega_0(n + 1/2)| \ll \hbar\omega_0$ and $\Gamma_n \ll \hbar\omega_0$, as is reasonable for weakly modulated high-mobility systems. Then, a typical contribution to the scattering conductivity is of the form

$$|(n, X|v_y|n \pm 1, X)|^2 A_n(E; X) A_{n \pm 1}(E; X)$$

with $E_n \approx E = E_F$, the Fermi energy. Here we may estimate

$$A_{n \pm 1}(E \approx E_n; X) \approx \Gamma_{n \pm 1}/[2\pi(\hbar\omega_0)^2].$$

On the other hand, the corresponding contribution to the band conductivity is

$$[(n, X|v_y|n, X) A_n(E_F; X)]^2.$$

Since $[A_n(E_F; X)]^2 \sim A_n(E_F; X) 2/[\pi\Gamma_n]$, the product of the spectral function factors is now by a factor $4(\hbar\omega_0)^2/(\Gamma_n \Gamma_{n \pm 1}) \sim 4(\omega_0 \tau)^2$ larger. Since for a mobility $\mu \geq 100 \text{ m}^2/\text{Vs}$ the product $\omega_0 \tau = \mu B \geq 10$ becomes large for $B > 0.1 \text{ T}$, the band conductivity can be very important even for a weak modulation $V(x) = V_0 \cos KX$, where according to Eqs. (40) and (35) the ratio of diagonal and off-diagonal velocity matrix elements can be estimated as $[KV_0/(m\omega_0)]/[l_0 \omega_0 \sqrt{2n+1}] \approx KR V_0/2E_F$, with $R = v_F/\omega_0$ the cyclotron radius at the Fermi energy.

Since the electrostatic modulation does not change the velocity operators, their matrix elements in the Landau representation are also not changed. As a consequence, the band conductivity does not show up explicitly in the formalism of Sec. II B. To clearly separate the band conductivity from the scattering conductivity, we work in the following in the energy eigenbasis $|n, X\rangle$ of the modulated system with the Hamiltonian of Eq. (1), the “ H representation.” However, we will consider only weak modulations, which we treat in lowest order perturbation expansion starting from the Landau basis of the unperturbed homogeneous system.

B. Basic approximation

Our simplified approach is based on the H -representation which allows to decompose the velocity operator

$$v_y = \sum_{m,n} |n, X\rangle \langle n, X| v_y |m, X\rangle \langle m, X| = v_y^{\text{dia}} + v_y^{\text{off}} \quad (42)$$

into a H -diagonal part v_y^{dia} defined by $\langle n, X| v_y^{\text{dia}} |n, X\rangle = \langle n, X| v_y |n, X\rangle$ and the remaining off-diagonal part v_y^{off} . The approximation scheme basically consists of three steps.

First, we assume that, for weak enough modulation, only the diagonal matrix elements $\langle n, X| G |n, X\rangle$ and $\langle n, X| \Sigma |n, X\rangle$ contribute essentially to the expectation values we want to calculate. Therefore, we approximate the self-energy to be diagonal in the eigenbasis of the Hamiltonian H . Then it follows from Eq. (2) that G is diagonal, too

$$\langle n, X| G^\sigma(E) |m, X\rangle = \delta_{n,m} G_n^\sigma(E; X). \quad (43)$$

This is exact for vanishing modulation and expected to be a very good approximation for weak modulation. In view of Ward identities such as Eq. (18), diagonality of G requires that the vertex operators should have the same matrix structure as the velocity operators. We come back to this requirement.

Second, we use lowest order perturbation theory, to express matrix elements in the H representation by those of the Landau representation. Thus, we approximate the energy spectrum by $E_n(X) = \langle n, X| H |n, X\rangle$,

$$E_n(X) = \epsilon_n + V_0 \mathcal{J}_{n,n} (l_0^2 K^2 / 2) \cos(KX), \quad (44)$$

with $\mathcal{J}_{n,n}$ defined in Eq. (A4), and the energy eigenstates by

$$|n, X\rangle = |n, X\rangle + \sum_{m(\neq n)} \frac{\langle m, X| V_0 \cos Kx |n, X\rangle}{\epsilon_n - \epsilon_m} |m, X\rangle, \quad (45)$$

but we keep the terms of first order in V_0 only if the terms of zeroth order vanish. To be specific, we calculate the diagonal matrix elements $v_{y;n,n}(X) = \langle n, X| v_y |n, X\rangle$ from Eq. (45) to first order in V_0 , obtaining Eq. (40) with $E_n(X)$ given by Eq. (44). For v_y^{off} , v_x , G , and Σ we use Eq. (45) to zeroth order in V_0 to replace the matrix elements in the H representation by the corresponding Landau matrix elements $v_{y;n,m}^{\text{off}} = \langle n, X| v_y |m, X\rangle$, $v_{x;n,m} = \langle n, X| v_x |m, X\rangle$, etc.

In the third and last step we approximate the SCBA kernel. First, we use Eq. (45) to replace the matrix elements of

the kernel in the H representation by the corresponding Landau matrix elements. This means that we neglect modulation effects on the “collision operator” describing the random impurity scattering. A similar approximation was made in the classical calculations,¹ where the collision operator of Boltzmann’s equation was taken as that of the unmodulated system. Next we note that, even if the Green operator is diagonal, the right-hand side of Eq. (15) still has off-diagonal entries. Requiring the self-energy to be diagonal, therefore means to neglect certain parts of the kernel. We make this neglect manifest by imposing selection rules similar to those in the homogeneous system, Eq. (33), and we replace $K_{k,l}^{n,m}(X)$ with (see Appendix A1)

$$\begin{aligned} \tilde{K}_{k,l}^{n,m}(X) &= \delta_{n-m, k-l} K_{k,l}^{n,m}(X) \\ &= \delta_{n-m, k-l} \sum_{\lambda} e^{i\lambda KX} \frac{n_i}{2\pi l_0^2} \int_0^\infty dQ |u_q|^2 \\ &\quad \times \mathcal{J}_{n,k}(Q) \mathcal{J}_{l,m}(Q) J_0(\lambda K l_0 \sqrt{2Q}). \end{aligned} \quad (46)$$

However, in contrast to the homogeneous system, we consider also the terms with $\lambda \neq 0$.

Within this approximation scheme the vertex operators defined in Eq. (7) have the same matrix structure as the corresponding components of the velocity operator. As a consequence, band and scattering conductivities can still be distinguished and the Ward identities are fulfilled (see Appendix B1). We call this approximation scheme the H -diagonal approximation (HDA).

C. Conductivity

The HDA contains several restrictive approximations in addition to the general SCBA formalism sketched in Sec. II B. Therefore, we have to make sure that the relevant Ward identities remain satisfied with the modified kernel (46). The self-energy is now determined by

$$\Sigma_n^\sigma(E; X) = \sum_m \int_0^a \frac{dX'}{a} \tilde{K}_{m,n}^{n,n}(X-X') G_m^\sigma(E; X'), \quad (47)$$

with $G_n^\sigma(E; X) = 1/[E - E_n(X) - \Sigma_n^\sigma(E; X)]$ (for $\sigma = \pm$).

The velocity matrix elements, which we denote by $v_{\nu;n,m}(X) = \langle n, X| v_\nu |m, X\rangle$, are taken in leading order of the modulation, which means zeroth order for the off-diagonal elements, being thus identical with the Landau matrix elements, and first order for the diagonal matrix elements. Because of Eq. (46) and the diagonality of the Green operator, the Bethe-Salpeter equation transfers the matrix structure of the velocity operator onto the vertex operator and the contribution of $v_{y;n,n}(X)$ to the conductivity can be separated from the contribution of the off-diagonal elements. Following Ref. 6, we call them band and scattering conductivities, σ_{yy}^{bd} , and $\sigma_{\nu\nu}^{\text{sc}}$ respectively.

The Bethe-Salpeter equation Eq. (13) now reads

$$F_{v;nm}^{\sigma\sigma'}(E;X) = G_n^\sigma \left\{ v_{v;n,m}(X) + \sum_{k,l} \int_0^a \frac{dX'}{a} \tilde{K}_{k,l}^{n,m}(X-X') F_{v;kl}^{\sigma\sigma'}(E;X') \right\} G_m^{\sigma'}, \quad (48)$$

where $F_{v;nm}^{\sigma\sigma'}(E;X)$ denote the approximated matrix elements of the vertex operators.

For the off-diagonal contributions, the derivation of the Ward identities is sketched in Appendix B. The diagonal components of the conductivity tensor are given by Eqs. (20) and (27), but since $A(E)$ is diagonal, the contributions of the anticommutator terms vanish. The vertex operators are determined by Eqs. (21) and (28), however, the integral operators are given by the reduced kernel (46) and, in our lowest order approximation, the term $\propto dV/dx$ in Eq. (28) is neglected. Due to the explicit form of the Landau matrix elements, Eq. (35), and the properties of the linear integral equations one finds that the scattering conductivities in the HDA are equal,

$$\sigma_{xx}^{\text{sc}}(E) = \sigma_{yy}^{\text{sc}}(E) = \frac{e^2 \hbar}{2\pi S} \text{Tr} v_x \tilde{F}_x^{+-}(E). \quad (49)$$

Thus, the longitudinal conductivities have the following structure:

$$\sigma_{xx} = \sigma_{xx}^{\text{sc}}, \quad (50)$$

$$\sigma_{yy} = \sigma_{xx}^{\text{sc}} + \sigma_{yy}^{\text{bd}}. \quad (51)$$

Next, we consider the band conductivity σ_{yy}^{bd} . The relevant Ward identity for the evaluation of the diagonal part of $v_x(F_y^{++} + F_y^{--})$ is the diagonal part of Eq. (A7). Now only the term with the X derivative survives, since due to the diagonality of G the commutator term is off-diagonal,

$$F_{y;nm}^{\sigma\sigma}(E;X) = -\frac{1}{m\omega_0} \frac{d}{dX} G_n^\sigma(E;X). \quad (52)$$

The resulting contribution to the band conductivity is

$$\delta\sigma_{yy}^{\text{bd}}(E) = -\frac{e^2 l_0^2 g_s}{8\pi^2 \hbar} \sum_n \int_0^a \frac{dX}{a} \frac{dE_n}{dX} \frac{d(G_n^- + G_n^+)}{dX}, \quad (53)$$

where $g_s=2$ accounts for spin degeneracy. Thus, the total band conductivity is given by

$$\sigma_{yy}^{\text{bd}}(E) = \delta\sigma_{yy}^{\text{bd}}(E) + \frac{e^2 \hbar^2 g_s}{(2\pi l_0)^2} \sum_n \int_0^a \frac{dX}{a} v_{y;n,n}(X) F_{y;n,n}^{+-}(E;X), \quad (54)$$

where the diagonal part of the vertex operator F_y^{+-} has to be calculated from the Bethe-Salpeter equation (48).

The Eqs. (31) and (32) for the Hall conductivities also simplify in the HDA. As we show in Appendix B2, they can be combined to

$$\sigma_{yx}^{\text{sc}}(E) = -\sigma_{xy}^{\text{sc}}(E) = \frac{e^2 \hbar}{2\pi\omega_0 S} \text{Tr} C_1[v_x] \tilde{F}_x^{+-}. \quad (55)$$

In summary, to calculate within the HDA all components of the conductivity tensor according to Eqs. (9) and (29), one has to solve in addition to the nonlinear Dyson equation for the (diagonal) Green operator two linear integral equations, namely, Eq. (21) for \tilde{F}_x^{+-} and the diagonal part of Eq. (48) for $F_{y;n,n}^{+-}(E;X)$. Of course, all results obtained within the HDA become exact (within the SCBA) in the limit of an unmodulated, homogeneous 2DES.

IV. NUMERICAL RESULTS

A. Characteristic examples

For numerical calculations we use the material parameters of GaAs ($m=0.067m_0$) and impurity potentials of Gaussian shape^{12,13}

$$u(r) = \frac{u_0}{\pi r_0^2} e^{-(r/r_0)^2}. \quad (56)$$

In the limit $r_0 \rightarrow 0$ this leads to a delta-like potential, which describes isotropic scattering, whereas with increasing r_0 forward scattering becomes predominant. For a quantitative comparison with experiments, we also consider a screened Coulomb potential with Fourier components

$$u_q = u_0 \frac{e^{-q|z|}}{q/q_{\text{TF}} + 1}, \quad (57)$$

where $q_{\text{TF}} = 2/a_B^*$, and $a_B^* \approx 10$ nm is the effective Bohr radius in GaAs. This is a better approximation to the potential induced by charged donors behind a spacer of thickness z .

In the following we examine the influence of the vertex corrections on the resistance of a modulated 2DES. As we have already demonstrated elsewhere,⁸ even in unmodulated systems the vertex corrections become important in the presence of anisotropic scattering. We were able to show that the garland like structures in the Hall resistance, which were calculated in early papers^{14,15} and have been observed in experiments on Si-MOSFET's inversion layers¹⁵⁻¹⁸ but never in GaAs heterostructures, are a typical effect of short-range impurity scattering and do not occur for long-range scattering potentials as those due to donors behind a spacer in typical AlGaAs heterostructures.

In Fig. 1 we compare the density of states (DOS) at the Fermi energy [$D(B)$, upper part] and the resistances (upper and middle part) for CNA and HDA. For the resistances we also include HDA calculations without vertex corrections. To characterize the impurity scattering, we have in principle three parameters, the density of impurities and strength and range of the impurity potential. Density and strength are combined in the "scattering strength" $\Gamma_0 = n_i u_0^2 m / (2\pi \hbar^2)$,

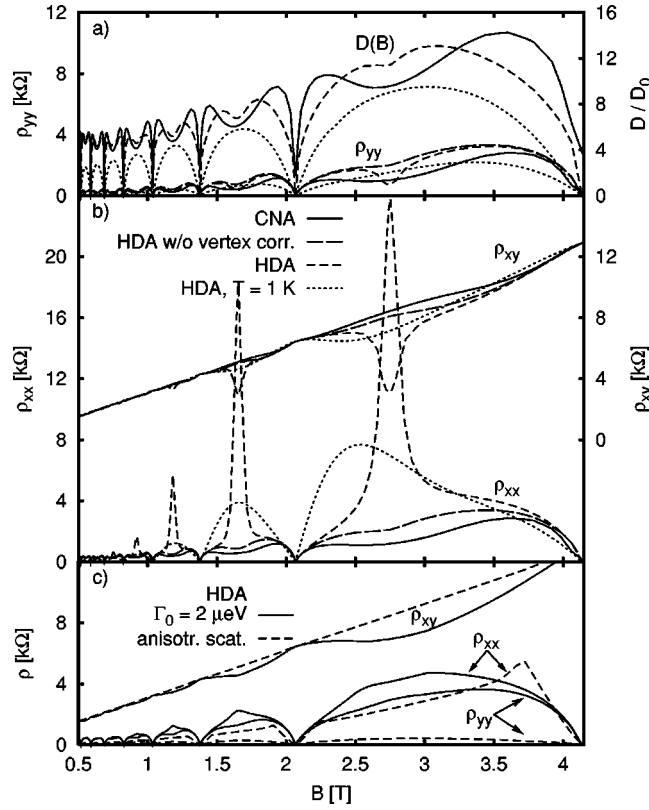


FIG. 1. (a) DOS at the Fermi energy $D(B)$ and resistivity ρ_{yy} and (b) resistivities ρ_{xy} and ρ_{xx} for different approximations assuming isotropic scattering with $\Gamma_0 = 1 \mu\text{eV}$ ($\rho_0 = 11\Omega$), and $V_0 = 0.16 \text{ meV}$, $a = 500 \text{ nm}$, $n_{\text{el}} = 2 \times 10^{15} \text{ m}^{-2}$, $T = 0 \text{ K}$. (c) Resistivities in HDA with the same values of V_0 , a , n_{el} , and T , for anisotropic scattering according to Eq. (56) with $r_0 = 20 \text{ nm}$ and $\Gamma_0 = 52 \mu\text{eV}$, i.e., $\rho_0 \approx 11\Omega$ (dashed lines) and for isotropic scattering with $\Gamma_0 = 2 \mu\text{eV}$, i.e., $\rho_0 = 23\Omega$ (solid lines).

which has the dimension energy. The range determines the transport (or momentum relaxation) time τ_{tr} ,

$$\frac{\hbar}{\tau_{\text{tr}}} = \Gamma_0 \int_{-\pi}^{\pi} d\varphi \left| \frac{u_q}{u_0} \right|_{q=k_F \sqrt{2-2\cos\varphi}}^2 (1 - \cos\varphi), \quad (58)$$

which enters the Drude formula for the conductivity (at $B_0 = 0$) of the unmodulated system, $\rho_0 = m/(e^2 \tau_{\text{tr}} n_{\text{el}})$. For extremely short-range potentials $u_q \approx u_0$ one has $\hbar/\tau_{\text{tr}} = 2\pi\Gamma_0$ and $\rho_0 = (h/e^2)\pi\Gamma_0/E_F$, with $E_F = n_{\text{el}}/D_0$ and $D_0 = g_s m/(2\pi\hbar^2) = 2.79 \times 10^{10} (\text{meV cm}^2)^{-1}$ the density of states of the 2DES in GaAs at $B_0 = 0$. With increasing range of the impurity potential $\hbar/(2\pi\Gamma_0\tau_{\text{tr}})$ decreases rapidly. For model (56), $\hbar/(2\pi\Gamma_0\tau_{\text{tr}}) = g[(k_F r_0)^2]$ is given by modified Bessel functions $g(\zeta) = \exp(-\zeta)[I_0(\zeta) - I_1(\zeta)]$.

Already in the DOS differences between the two approximations show up. The van Hove singularities are much less pronounced in HDA than in CNA and the band edges are more rounded. But these subtleties are no longer visible at higher temperatures. On the other hand, the peak height is similar in both approximations.

This is no longer true for ρ_{yy} , the ‘‘scattering resistance.’’ In the upper magnetic field range ($2.5 \lesssim B/T < 3.4$), CNA

and HDA without vertex corrections differ by a factor of about 2. Apparently the vertex corrections lower the scattering resistance significantly in the center of the Landau band, where the dispersion is maximum. An increase of temperature smears out this dip and at 1 K the vertex corrections lead to a lowering of ρ_{yy} everywhere (not only in the center).

As seen in Fig. 1(b), the effect of vertex corrections on the band conductivity is much more drastic. In CNA and HDA without vertex corrections, ρ_{xx} and ρ_{yy} differ only marginally, since the band conductivity is almost zero. But in the full HDA, there are huge contributions of the band conductivity to ρ_{xx} exceeding the scattering conductivity by a factor of 4 at high magnetic fields. These peaks increase rapidly with the magnetic field as they depend sensitively on the dispersion, which is high for low Landau indices and far away from the flat-band conditions,⁶ at which the width of the modulation broadened Landau bands shrinks to zero [$\mathcal{J}_{n,n}(l_0^2 K^2/2) \approx 0$, see Eq. (44)]. The peculiar shapes of the bands are caused by the superposition of broad scattering contributions and large, narrow peaks due to the band conductivity. Again, such structures vanish rapidly with increasing temperature. The dips in the Hall resistance result, after tensor inversion, from the large values of σ_{yy} .

Not only the energy dispersion but also the broadening of the Landau bands due to scattering influences the magnitude of the vertex corrections strongly. In the lower part of Fig. 1 the resistances are plotted for a higher scattering strength Γ_0 (solid lines), corresponding to a larger ρ_0 . For such a line broadening the van Hove singularities are no longer visible in DOS and ρ_{yy} . The increase of Γ_0 by a factor of 2 leads only to a weak increase of the scattering conductivity, but the drastic reduction of ρ_{xx} shows the sensitive dependences of the band conductivity on the scattering strength. Therefore, the difference between ρ_{xx} and ρ_{yy} vanishes rapidly.

The anisotropy of the impurity scattering is another parameter which influences the ratio of ρ_{xx} and ρ_{yy} greatly. In the lower part of Fig. 1 also the resistances for anisotropic scattering with $r_0 = 20 \text{ nm}$ are plotted (dashed lines) with the same zero-field resistance ρ_0 as in the situation of the upper panel. For given ρ_0 the scattering strength Γ_0 must be chosen much higher in the anisotropic case than in the isotropic one. Consequently, the band conductivity is much smaller. But at the same time, anisotropic scattering leads to a much weaker increase of the scattering resistance with magnetic field. This means, in the high magnetic field range there is still a considerable anisotropy between ρ_{xx} and ρ_{yy} for anisotropic scattering, as opposed to the situation we considered before, where Γ_0 was only slightly increased but r_0 was held constant. In the Hall resistance the garlandlike structures vanish as in the homogenous system.⁸

This discussion shows that even for isotropic scattering the vertex corrections, which are neglected in the c-number approximation, lead to important contributions to the band conductivity if the scattering rate is not too high. We now discuss the case of anisotropic scattering in more detail as it is important for interpreting experiments in GaAs heterostructures.

B. Comparison with experimental results

Classical calculations can explain the commensurability oscillations¹⁹ of ρ_{xx} (also called “Weiss oscillations”) both for isotropic and for anisotropic scattering. The antiphase oscillations in ρ_{yy} and the Shubnikov–de Haas (SdH) oscillations, on the other hand, are of a purely quantum mechanical origin. They are dominated by the DOS, which shows modulation-induced amplitude oscillations owing to the oscillatory (n and B dependent) width of the Landau levels. As has been discussed in detail in Ref. 6, within the CNA the scattering conductivity, which dominates ρ_{yy} , is given by the thermal average of the square of the DOS, and exhibits the commensurability oscillations to much higher temperatures than the thermodynamic DOS. Within the HDA the relation between scattering conductivity and DOS is not so obvious due to the vertex corrections, but Fig. 1(a) shows clearly that the oscillations of ρ_{yy} still follow closely those of $D(B)$. The CNA, which includes these quantum effects, is however only in a rough qualitative agreement with experiments and has to rely on an unrealistic choice of system parameters which can reproduce some aspects of the experiment at the price of a disagreement with others. If, e.g., the damping is chosen small enough to reproduce the zero-field resistance, the width of the Landau levels comes out too small, i.e., the amplitude of the SdH oscillations comes out too large.⁶ If, on the other hand, the latter are fitted well, the zero-field resistance comes out much too large. We now give an example showing that a correct treatment of the vertex corrections can yield a nearly quantitative agreement with experiment for all oscillatory quantum effects. To do so, we compare with an early experiment by D. Weiss *et al.* [Fig. 3 of Ref. 19(a), Fig. 2 of Ref. 19(b), and Fig. 6.1 of Ref. 19(c)] and choose a weak modulation strength, $V_0=0.45$ meV, in agreement with a previous estimate¹⁹ based on the maximum of the largest commensurability peak. The only adjustable parameter is the scattering anisotropy, which cannot be determined so easily from the experiment.

In Fig. 2 the resistances for parameters similar to the experimental situation¹⁹ are plotted for different ranges of the impurity potential. The solid lines in the upper panel denote ρ_{xx} and ρ_{yy} in CNA. They show strong oscillations, upon which at higher field values SdH oscillations are superimposed. At the flat-band conditions ρ_{yy} , which is dominated by the scattering conductivity, shows maxima as expected. Taking the difference $\rho_{xx}-\rho_{yy}$ as a measure for the band conductivity, this shows also the expected Weiss oscillations of opposite phase, with minima at the flat-band conditions. But apparently the amplitude of the scattering conductivity oscillations is much larger than that of the band conductivity oscillations, so that ρ_{xx} exhibits maxima at the flat-band conditions, which are caused by the scattering conductivity, instead of the expected minima. These findings are not in agreement with the experimental observations. Also the average increase of the longitudinal resistances with increasing magnetic field is much stronger for the CNA results than in the experiment. The amplitudes of the Weiss oscillation increase linearly with magnetic field, in correspondence to

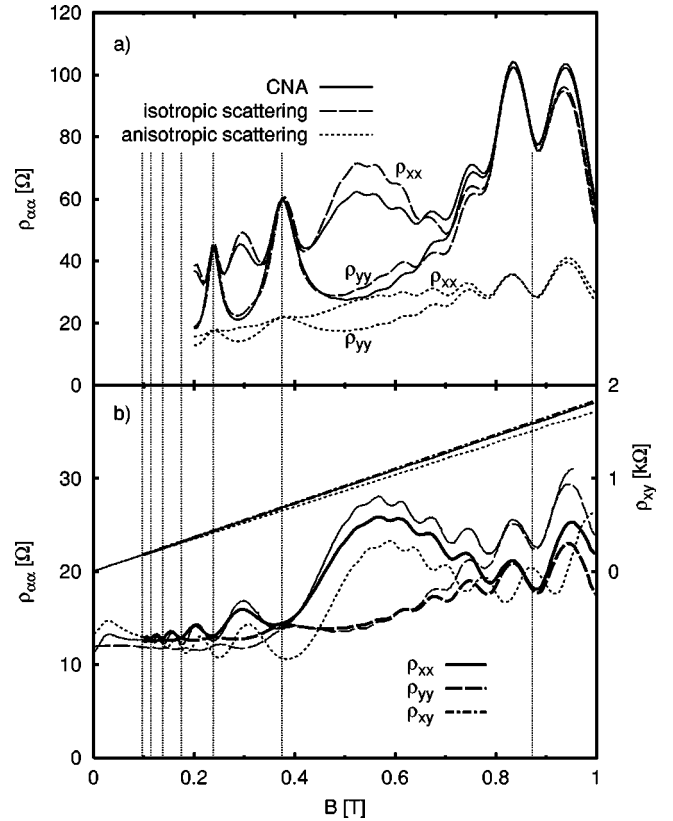


FIG. 2. Effect of scattering anisotropy. (a) Resistivities for isotropic scattering in CNA and in HDA both with $\Gamma_0=1.85 \mu\text{eV}$, and for anisotropic scattering in HDA with $r_0=15$ nm and $\Gamma_0=92.5 \mu\text{eV}$, yielding all $\rho_0=12.3\Omega$. (b) Thick lines: calculated resistivities for Coulomb scattering, Eq. (57), with $z=14$ nm, $\Gamma_0=0.8$ meV, i.e., $\rho_0=12\Omega$. Remaining parameters in (a) and (b) $T=4.2$ K, $n_{el}=3.4\times 10^{15} \text{ m}^{-2}$, $V_0=0.45$ meV, $a=294$ nm. The vertical lines indicate the minima of the Weiss oscillations (flat-band conditions). Thin lines: experimental results after Ref. 19 (see text).

classical calculations for isotropic scattering,¹ but in disagreement with the experiment.¹⁹

Here we should comment on an apparent error in the results of Ref. 6, which can not be reproduced as has been asserted by several independent workers.²⁰ For the given parameter values the oscillatory scattering conductivity obtained in Ref. 6 seems too small as compared with the band conductivity. We obtain for their parameter values a result similar to the CNA calculation in Fig. 2(a), where the oscillations of the scattering conductivity are larger than those of the band conductivity, and lead to pronounced in-phase maxima of ρ_{xx} and ρ_{yy} at the flat-band conditions.

Including vertex corrections within a HDA calculation for isotropic scattering [broken lines in Fig. 2(a)] does not change the CNA picture qualitatively. We now consider anisotropic scattering due to finite-range impurity potentials (dotted lines), leading to the same zero-field resistance ρ_0 . This results in a slower increase of the resistances with the magnetic field. But at the same time the oscillation amplitudes decrease drastically. This effect is stronger for the antiphase oscillations of the scattering conductivity than for the

Weiss oscillations and causes the unexpected structure in ρ_{xx} to vanish. Obviously the scattering anisotropy is an important parameter for describing the experimental situation.

For the lower part of Fig. 2 we tried to adjust the anisotropy to get close agreement with the experiment. Here we used the screened Coulomb potential, which leads to a ratio of band and scattering conductivity corresponding more closely to the experimental findings. The calculated conductivities are shown by thick lines, as indicated in the legend of Fig. 2(b). Also shown are experimental results¹⁹ obtained from holographic modulation of an L -shaped sample. The thin long-dashed line for ρ_{yy} and the thin solid line for ρ_{yx} are measured in that leg of the sample, where the current flows parallel to the equipotentials of the modulation. The dotted lines for ρ_{xx} (lower oscillating line) and for ρ_{xy} (upper nearly straight line) are taken from the other leg where the current flows perpendicular to the equipotentials. From both the position of the SdH minima and the Hall resistivity we conclude that in this leg the electron density is about 4% larger than in the other leg. Moreover, the oscillations of ρ_{xx} seem to be superimposed on a slowly varying, quasiparabolic background, which is attributed by the experimentalists¹⁹ to the effect of sample inhomogeneities, and is not taken into account in our theory. To correct for these effects, we first interpret the horizontal (B) axis as a $1/\nu$ axis (with ν the Landau level filling factor $B[T]=14.1/\nu$) and reduce the abscissa values of the dotted curves by the factor 0.96, so that the positions of the SdH minima coincide with those of ρ_{yy} and the ρ_{xy} practically coincides with the ρ_{yx} trace. (Due to this scaling the flat-band conditions shift to marginally lower values, by about 2%.) Then we tentatively subtract from the scaled ρ_{xx} curve the smooth background $\Delta\rho_{xx}[\Omega]=2-19x+12.5x^2$, with $x=B[T]$, and obtain the thin solid line as the corrected ρ_{xx} curve. Apart from a smooth quasiparabolic increase at large B values (probably still due to inhomogeneities), the agreement between theory and experiment is now very good, at least in the regime $0.1\text{ T}<B<1\text{ T}$ which is determined by the commensurability and the SdH oscillations. The amplitudes of the Weiss oscillations decrease with decreasing B much faster than linearly, in agreement with classical calculations^{1,2,21,22} for anisotropic impurity scattering. The positive magnetoresistance at very small B values is well understood from classical calculations.^{1,22} The garland-like structures in the Hall resistance of previous calculations^{14,15} are suppressed by anisotropic scattering, as in the homogenous system.

V. SUMMARY

We have developed an approximation scheme for weak modulation potentials and showed that it is consistent with Ward identities. This “ H -diagonal approximation” (HDA) can be summarized as follows. We work in the energy eigenbasis $|n, X\rangle$ of the Hamiltonian H including the modulation, Eq. (1), and assume that self-energy and, consequently, Green operator are diagonal. In the spirit of a lowest order perturbation expansion with respect to the modulation potential $V(x)=V_0\cos Kx$, we calculate energy spectrum $E_n(X)$ and diagonal elements of the velocity $\langle n, X|v_y|n, X\rangle=$

$-(m\omega_0)^{-1}dE_n(X)/dX$ up to first order in V_0 . On the other hand, we neglect the modulation in the off-diagonal components of the velocity operators and in the collision operator describing random impurity scattering, i.e., we replace their matrix elements by the corresponding matrix elements in the Landau representation. To achieve consistency, we imposed selection rules on the collision operator, similar to those valid in homogeneous systems.

Our approximation scheme allows the separation of band and scattering conductivities, giving rise to a simple explanation of Weiss and antiphase oscillations as in previous calculations using a c -number approximation (CNA) for the self-energy. On the other hand, it does not suffer from the problems of the CNA. For the calculation of the conductivity tensor two transport equations have to be solved, one for the scattering and the Hall conductivities, and another one for the band conductivity. Furthermore, the HDA includes anisotropic scattering. Numerical comparisons have shown that the corrections due to the Ward identities give important contributions especially to the band conductivity, and in the high magnetic field range even for isotropic scattering.

We showed that, with a correct treatment of small-angle scattering, quantum mechanical transport calculations are able to reproduce the experimental results with a minimum number and realistic values of material parameters to a very high quantitative accuracy. Contrary to classical calculations not only the Weiss oscillations of ρ_{xx} but also the antiphase of ρ_{yy} and the SdH oscillations are obtained. Furthermore, we obtain realistic results for the Hall resistance and not the garlandlike structures which are typical for isotropic impurity scattering.⁸

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APPENDIX A: SCBA RESULTS

1. SCBA kernel

Inserting the Fourier expansion

$$G_{n,m}^{\pm}(E;X)=\sum_{\lambda}\exp(i\lambda KX)G_{\lambda;n,m}^{\pm}(E)$$

into Eq. (11) and calculating the Fourier coefficient $\Sigma_{\lambda;n,m}^{\pm}(E)$, we obtain with Eq. (12) for the Fourier coefficients of the general kernel

$$\begin{aligned} K_{n',m'}^{n,m}(\lambda;\lambda') &= \int_0^a \frac{dX}{a} \sum_{k'_y} e^{-i\lambda KX} n_i \int d^2R \langle n, X|u(\mathbf{r}-\mathbf{R})|n', X'\rangle \\ &\times e^{i\lambda' KX'} \langle m', X'|u(\mathbf{r}-\mathbf{R})|m, X\rangle \end{aligned} \quad (\text{A1})$$

$$= \delta_{\lambda',\lambda} \frac{n_i}{S} \sum_{\mathbf{q}} |u_{\mathbf{q}}|^2 e^{-i\lambda l_0^2 K q_y} \mathcal{L}_{n,n'}(\mathbf{q}) \mathcal{L}_{m',m}(-\mathbf{q}), \quad (\text{A2})$$

where $l_0 = \sqrt{\hbar/m\omega_0}$. Here we have inserted the Fourier transform $u_{\mathbf{q}} = \int_S d^2r u(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$ of the impurity potential, introduced intermediate states of the form $|n', X' = -l_0^2 k_y'\rangle$, and taken into account the properties of the matrix elements²³

$$\langle n, X | e^{i\mathbf{q}\cdot\mathbf{r}} | n', X' \rangle = \delta_{k_y, k_y' + q_y} e^{-iq_x(X+X')/2} \mathcal{L}_{n,n'}(\mathbf{q}),$$

in order to perform the integrations over the impurity positions \mathbf{R} and the center coordinates X . Assuming rotationally invariant impurity potentials, $u_{\mathbf{q}} = u_q$, we can replace the \mathbf{q} sum by an integral and perform its angular part to obtain for the kernel $K_{k,l}^{\lambda;n,m} \equiv K_{k,l}^{n,m}(\lambda; \lambda)$:

$$K_{k,l}^{\lambda;n,m} = i^{|n-k|-|l-m|} \frac{n_i}{2\pi l_0^2} \int_0^\infty dQ |u_q|^2 \times \mathcal{J}_{n,k}(Q) \mathcal{J}_{l,m}(Q) J_{k-l-n+m}(\lambda K l_0 \sqrt{2Q}), \quad (\text{A3})$$

$$\mathcal{J}_{n,m}(Q) = \frac{\min(n,m)!}{\sqrt{n!m!}} Q^{(1/2)|n-m|} e^{(1/2)Q} L_{\min(n,m)}^{|n-m|}(Q), \quad (\text{A4})$$

where $q = |\mathbf{q}| = \sqrt{2Q}/l_0^2$ and $L_\alpha^n(Q)$ denotes the Laguerre polynomials²⁴ and $J_n(x)$ the Bessel functions.^{9,23} Apparently

$$K_{k,l}^{\lambda;n,m} = K_{l,k}^{\lambda;m,n} = K_{n,m}^{-\lambda;k,l}. \quad (\text{A5})$$

Equivalent results have been obtained in Ref. 5, Appendix A.

2. Ward and related identities in SCBA

In order to evaluate the contribution of $F_y^{\sigma\sigma}$ to σ_{yy} we cannot proceed as for the x components, since there exists no analog of Eq. (17) for the y component of the position operator. Moreover, commutators including the position operator $r_y \equiv y$ must be handled with great care, first since the matrix elements of y in the Landau representation are ill defined, second because naive application of the cyclic invariance of the trace may lead to unjustified manipulations of divergent sums and invalid result. To avoid such problems, we may work in the momentum representation, where $y = i\hbar \partial/\partial p_y$ and the y component of Eq. (10) reads

$$F_y^{\sigma\sigma} = \partial G^\sigma(E) / \partial p_y. \quad (\text{A6})$$

To evaluate the Landau matrix elements of this expression, we take the derivative of $\langle m, X | G^\sigma(E) | n, X \rangle$ with respect to $X = -l_0^2 p_y / \hbar$. Calculating the derivatives of the Landau wave functions $\partial \langle x | n, X \rangle / \partial X$ directly from the Hermite polynomials, we obtain

$$\langle m, X | F_y^{\sigma\sigma} | n, X \rangle = -\frac{1}{m\omega_0} \frac{d}{dX} \langle m, X | G^\sigma | n, X \rangle - \frac{i}{\hbar\omega_0} \langle m, X | [G^\sigma, v_x] | n, X \rangle. \quad (\text{A7})$$

Evaluating contributions of the form

$$\frac{1}{S} \text{Tr} v_y F_y^{\sigma\sigma} = \frac{g_s}{2\pi l_0^2} \sum_{n,m} \int_0^a \frac{dX}{a} \langle n, X | v_y | m, X \rangle \langle m, X | F_y^{\sigma\sigma} | n, X \rangle \quad (\text{A8})$$

and noting that the velocity matrix elements are independent of X , we see that the contribution due to the X derivative in Eq. (A7) is the integral of the derivative of a periodic function of X over a full period a , and thus vanishes. Therefore, we obtain Eq. (25) as an analog of Eq. (18) and proceed as for σ_{xx} to derive Eq. (27).

Several other useful identities follow directly from the form (12) of the SCBA integral operator. Using the identity $[v_\mu, u(\mathbf{r}-\mathbf{R})] = (i\hbar/m) \partial u(\mathbf{r}-\mathbf{R}) / \partial R_\mu$ we obtain for $\mu \in \{x, y\}$

$$\begin{aligned} \Sigma^\sigma v_\mu - I[G^\sigma v_\mu] &= -\frac{i\hbar n_i}{m} \int d^2R u(\mathbf{r}-\mathbf{R}) G^\sigma \frac{\partial u}{\partial R_\mu} \\ &= v_\mu \Sigma^\sigma - I[v_\mu G^\sigma], \end{aligned} \quad (\text{A9})$$

where we have integrated by parts with respect to R_μ and assumed that the boundary terms vanish in the limit of large sample area. As an immediate consequence we note the identity

$$[\Sigma^\sigma, v_\mu] = I[[G^\sigma, v_\mu]], \quad (\text{A10})$$

which for $\mu = y$ follows for $r_y = x$ from Eqs. (14) and (17). According to Eq. (24), this implies $C_2[v_\mu] = 0$, i.e., $C[v_\mu] = C_1[v_\mu]$.

From the cyclic invariance of the trace, one has further

$$\text{Tr} O_1 I[O_2] = \text{Tr} O_2 I[O_1]. \quad (\text{A11})$$

Combining this with Eq. (A9), one derives

$$\begin{aligned} \text{Tr} G^{\sigma'}(E') (\{\Sigma^\sigma(E), v_\mu\} - I[\{G^\sigma(E), v_\mu\}]) \\ = -\text{Tr} G^\sigma(E) (\{\Sigma^{\sigma'}(E'), v_\mu\} - I[\{G^{\sigma'}(E'), v_\mu\}]), \end{aligned} \quad (\text{A12})$$

and, with arguments similar to those leading to Eq. (A9) but including second derivatives with respect to the components of \mathbf{R} ,

$$\begin{aligned} \text{Tr}[G^{\sigma'}(E'), v_\nu] (\{\Sigma^\sigma(E), v_\mu\} - I[\{G^\sigma(E), v_\mu\}]) \\ = \text{Tr}[G^\sigma(E), v_\nu] (\{\Sigma^{\sigma'}(E'), v_\mu\} - I[\{G^{\sigma'}(E'), v_\mu\}]). \end{aligned} \quad (\text{A13})$$

Using this for $v_\nu = v_x$, we obtain with Eq. (A7) finally

$$\begin{aligned} & \text{Tr} \frac{\partial G^{\sigma'}(E')}{\partial p_y} (\{\Sigma^\sigma(E), v_\mu\} - I[\{G^\sigma(E), v_\mu\}]) \\ &= \text{Tr} \frac{\partial G^\sigma(E)}{\partial p_y} (\{\Sigma^{\sigma'}(E'), v_\mu\} - I[\{G^{\sigma'}(E'), v_\mu\}]), \end{aligned} \quad (\text{A14})$$

where we have evaluated derivatives with respect to X explicitly in the Landau representation under due consideration of the symmetry properties (16) of the SCBA kernel.

3. Hall conductivities

Arguing as for the derivation of Eq. (25) [see below Eq. (A8)], we may write the contribution of Eq. (5) to σ_{xy} as

$$\phi_{xy}^{(1)}(E) = \text{Tr} v_x \left[2\tilde{F}_y^{+-} - \frac{2\pi}{\hbar\omega_0} \{v_x, A(E)\} \right]. \quad (\text{A15})$$

The contribution $\phi_{xy}^{(2)}(E)$ of Eq. (6) contains the operators D_y^σ which, according to their definition (8) and the Bethe-Salpeter equation (13), satisfy the linear integral equation

$$D_\mu^\sigma = G^\sigma (\Gamma_\mu^\sigma + I[D_\mu^\sigma]) G^\sigma, \quad (\text{A16})$$

where the inhomogeneity has been written in the form

$$G\Gamma_\mu^\sigma G = \frac{dG}{dE} G^{-1} F_\mu^{\sigma\sigma} - F_\mu^{\sigma\sigma} G^{-1} \frac{dG}{dE}. \quad (\text{A17})$$

In Eq. (A17) we have omitted the energy argument and the superscript σ of the Green operators.

We now show that, for the calculation of $\phi_{xy}^{(2)}(E)$, we do not need to solve Eq. (A16) for D_y^σ . To this end we derive from Eq. (1)

$$i\hbar\omega_0 v_x = [v_y, H] = [(G^\sigma)^{-1} + \Sigma^\sigma, v_y] \quad (\text{A18})$$

and write (again suppressing the superscripts σ)

$$\begin{aligned} i\hbar\omega_0 \text{Tr} v_x D_y &= \text{Tr} \{ [G^{-1}, v_y] G (\Gamma_y + I[D_y]) G + [\Sigma, v_y] D_y \} \\ &= \text{Tr} \{ [v_y, G] (\Gamma_y + I[D_y]) + [\Sigma, v_y] D_y \}. \end{aligned} \quad (\text{A19})$$

The last two terms in Eq. (A19) cancel because of Eqs. (A11) and (A10). Consequently,

$$i\hbar\omega_0 \text{Tr} v_x D_y^\sigma = \text{Tr} [v_y, G^\sigma] \Gamma_y^\sigma = \text{Tr} v_y [G^\sigma, \Gamma_y^\sigma], \quad (\text{A20})$$

and $\phi_{xy}^{(2)}(E)$ can be expressed completely in terms of the Green operator.

Next we show that σ_{xy} can be written in the form of Eq. (29). To do so we use Eqs. (A17) and (A6) together with $dG/dE = -G(1 - d\Sigma/dE)G$ and

$$v_y = \frac{i}{\hbar} [H, y] = \frac{\partial H}{\partial p_y} = -\frac{\partial G^{-1}}{\partial p_y} - \frac{\partial \Sigma}{\partial p_y}, \quad (\text{A21})$$

which can also be written as

$$\frac{\partial G}{\partial p_y} = -G \frac{\partial G^{-1}}{\partial p_y} G = G \left(v_y + \frac{\partial \Sigma}{\partial p_y} \right) G, \quad (\text{A22})$$

to obtain

$$[G, \Gamma_y] = 2 \frac{\partial G}{\partial p_y} + \left\{ v_y, \frac{dG}{dE} \right\} + \left\{ \frac{dG}{dE}, \frac{\partial \Sigma}{\partial p_y} \right\} - \left\{ \frac{\partial G}{\partial p_y}, \frac{d\Sigma}{dE} \right\}. \quad (\text{A23})$$

The contribution of the first term on the right-hand side to $\phi_{xy}^{(2)}(E)$ is, according to Eq. (A7) and the arguments on the explicit X dependence of the factors leading to Eq. (25),

$$\begin{aligned} & \frac{-i}{\hbar\omega_0} \text{Tr} v_y 2 \frac{\partial}{\partial p_y} (G^- - G^+) \\ &= \frac{-4\pi i}{(\hbar\omega_0)^2} \text{Tr} v_y [A(E), v_x] = -\frac{4\pi}{m\hbar\omega_0} \text{Tr} A(E). \end{aligned}$$

The corresponding contribution to the Hall conductivity is $\sigma_{xy}^{(0)} = -e^2 n_{\text{el}} / (m\omega_0)$. The contribution of the second term in Eq. (A23) to $\phi_{xy}^{(2)}(E)$ is

$$\frac{-i}{\hbar\omega_0} \text{Tr} v_y \left\{ v_y, \frac{d(G^- - G^+)}{dE} \right\} = \frac{d}{dE} \frac{4\pi}{\hbar\omega_0} \text{Tr} v_y^2 A(E). \quad (\text{A24})$$

The contribution due to the last two terms of Eq. (A23) can also be written as a total energy derivative

$$\begin{aligned} & \frac{-i}{\hbar\omega_0} \text{Tr} v_y \left(- \left\{ \frac{\partial G}{\partial p_y}, \frac{d\Sigma}{dE} \right\} + \left\{ \frac{dG}{dE}, \frac{\partial \Sigma}{\partial p_y} \right\} \right) \\ &= \frac{i}{\hbar\omega_0} \text{Tr} \frac{\partial G}{\partial p_y} \left(\left\{ \frac{d\Sigma}{dE}, v_y \right\} - I \left[\left\{ \frac{dG}{dE}, v_y \right\} \right] \right) \\ &= \frac{d}{dE} \frac{i}{2\hbar\omega_0} \text{Tr} \frac{\partial G}{\partial p_y} (\{\Sigma, v_y\} - I[\{G, v_y\}]). \end{aligned}$$

To see the last equality, we take the derivative of identity (A14) with respect to E' and then put $E' = E$ (and $\sigma' = \sigma$). Collecting terms we obtain Eq. (31), where we again used identity (A14), but now with $E' = E$ and $\sigma' = -\sigma$.

The evaluation of σ_{yx} follows similar lines. First we use Eqs. (A16) and (A21) to eliminate D_x^σ ,

$$\text{Tr} v_y D_x^\sigma = \text{Tr} \frac{\partial G^\sigma}{\partial p_y} \Gamma_x^\sigma. \quad (\text{A25})$$

With Eqs. (18) and (A22) we then obtain

$$\begin{aligned} \text{Tr} v_y D_x &= \frac{i}{\hbar\omega_0} \text{Tr} \left[\frac{\partial G}{\partial p_y} \left(2v_y - \left\{ \frac{d\Sigma}{dE}, v_y \right\} \right) \right. \\ &\quad \left. + \left(v_y + \frac{\partial \Sigma}{\partial p_y} \right) \left\{ \frac{dG}{dE}, v_y \right\} \right], \end{aligned} \quad (\text{A26})$$

and proceed as above to derive Eq. (32).

APPENDIX B: HDA RESULTS

1. Ward identities

Since within the HDA G is diagonal, the off-diagonal part of Eq. (A7) reduces to

$$F_y^{\text{off};\sigma\sigma} = -\frac{i}{\hbar\omega_0}[G^\sigma, v_x], \quad (\text{B1})$$

similar to Eq. (18), whereas the diagonal part yields Eq. (52).

To prove that both Eqs. (18) and (B1) hold within the HDA, we have to show (for $\nu=x, y$)

$$[\Sigma^\sigma(E), v_\nu] = I[[G^\sigma(E), v_\nu]]. \quad (\text{B2})$$

Inserting the explicit velocity matrix elements, Eq. (35), and performing a Fourier transformation of $\Sigma_n^\sigma(E; X)$ and $G_n^\sigma(E; X)$ with respect to X , we find that, in order to prove Eq. (B2) for both $\nu=x$ and $\nu=y$, it is sufficient to show that

$$\begin{aligned} & [\Sigma_n^{\lambda;\sigma}(E) - \Sigma_m^{\lambda;\sigma}(E)]\sqrt{2n+1+\epsilon}\delta_{m,n+\epsilon} \\ &= \sum_{k,l} \tilde{K}_{k,l}^{\lambda;n,m}[G_k^{\lambda;\sigma}(E) - G_l^{\lambda;\sigma}(E)]\sqrt{2k+1+\epsilon}\delta_{l,k+\epsilon} \end{aligned} \quad (\text{B3})$$

holds for $\epsilon=\pm 1$, where the symbols with superscript λ denote the Fourier transforms of the actual quantity. With Dyson's equation in the HDA,

$$\Sigma_n^{\lambda;\sigma}(E) = \sum_k \tilde{K}_{k,k}^{\lambda;n,n} G_k^{\lambda;\sigma}(E), \quad (\text{B4})$$

and a relabeling in the last sum of Eq. (B3), we find that Eq. (B3) holds if the kernel of the HDA satisfies the consistency relation

$$\begin{aligned} & \sqrt{2n+1+\epsilon}(\tilde{K}_{k,k}^{\lambda;n,n} - \tilde{K}_{k,k}^{\lambda;n+\epsilon,n+\epsilon}) \\ &= \sqrt{2k+1+\epsilon}\tilde{K}_{k,k+\epsilon}^{\lambda;n,n+\epsilon} - \sqrt{2k+1-\epsilon}\tilde{K}_{k-\epsilon,k}^{\lambda;n,n+\epsilon}. \end{aligned} \quad (\text{B5})$$

The validity of this equation is seen with the definition of the HDA kernel, Eq. (46), and the recursion relations of the Laguerre polynomials.²⁴

To demonstrate that the diagonal Ward identity (52) holds within our HDA, we express the left-hand side by the Bethe-Salpeter equation (48) and calculate the right-hand side from Dyson's equation. Then, Eq. (52) is seen to be equivalent with the derivative of Eq. (15) with respect to X .

2. Hall conductivity in HDA

Since v_x and $F_x^{\sigma\sigma'}$ are off-diagonal, only the off-diagonal parts of v_y and $F_y^{\sigma\sigma'}$ contribute to the Hall conductivities in Eqs. (31) and (32). In the HDA the second term on the right-hand side of Eq. (31) vanishes, since $A(E)$ is diagonal

and $v_x^2 - v_y^2 = (v_+^2 + v_-^2)/2$ has no diagonal elements. Due to Eqs. (21) and (28), where the higher order term $\propto dV/dx$ has to be neglected in the HDA, and in view of Eqs. (35) and (46), we can write

$$\tilde{F}_x^{+-} = \frac{i}{2}(F_+ - F_-), \quad \tilde{F}_y^{+-} = \frac{1}{2}(F_+ + F_-), \quad (\text{B6})$$

where the auxiliary operators F_\pm satisfy

$$F_\pm - G^+ I[F_\pm] G^- = G^+ C_1[v_\pm] G^- \quad (\text{B7})$$

and have the same matrix structure as the velocity operators v_\pm . As a consequence, we find

$$\text{Tr } v_x \tilde{F}_y^{+-} = \frac{1}{4} \text{Tr}(v_+ F_- + v_- F_+) = -\text{Tr } v_y \tilde{F}_x^{+-}, \quad (\text{B8})$$

and therefore, with Eqs. (31) and (32),

$$\begin{aligned} \sigma_{yx}^{\text{sc}}(E) &= -\sigma_{xy}^{\text{sc}}(E) \\ &= \frac{e^2 \hbar}{2\pi S} \text{Tr} \left(v_y \tilde{F}_x^{+-} - \frac{i}{\hbar\omega_0} (G^- v_x - v_x G^+) C_1[v_y^{\text{off}}] \right). \end{aligned} \quad (\text{B9})$$

To obtain the last line from Eq. (32), we have replaced $\partial(G^- + G^+)/\partial p_y$ with its off-diagonal part in the HDA, $-i[(G^- + G^+), v_x]/(\hbar\omega_0)$ [see Eqs. (A7) and (B1)], to which we have added $-i[(G^- - G^+), v_x]/(\hbar\omega_0)$ without changing the value of the trace, since in the HDA

$$\text{Tr}\{A, v_x\} C_1[v_y^{\text{off}}] = \frac{1}{8i\hbar} \text{Tr}[v_+, v_-][A, \Gamma] = 0. \quad (\text{B10})$$

The trace of the last term in Eq. (B9) can be evaluated as

$$\begin{aligned} & -\frac{i}{\hbar\omega_0} \text{Tr } G^- ([H, v_x] + \Sigma^- v_x - v_x \Sigma^+) G^+ C_1[v_y^{\text{off}}] \\ &= -\frac{i}{\hbar\omega_0} \text{Tr}([H, v_x] + \Sigma^- v_x - v_x \Sigma^+) \\ & \quad \times (G^+ I[\tilde{F}_x^{+-}] G^- - \tilde{F}_x^{+-}) \\ &= -\frac{i}{\hbar\omega_0} \text{Tr}\{[I[G^- v_x - v_x G^+] - (\Sigma^- v_x - v_x \Sigma^+)] \\ & \quad \times \tilde{F}_x^{+-} - [H, v_x] \tilde{F}_x^{+-}\}. \end{aligned}$$

In the second version of the equation we have used Eq. (21). The last term cancels $v_y \tilde{F}_x^{+-}$ in Eq. (B9), since in the equation $[v_x, H] = -i\hbar\omega_0 v_y - i(\hbar/m)dV(x)/dx$ [see Eq. (1)] we have to neglect the term including $dV(x)/dx$ in our lowest order HDA. The term in the curly brackets equals $-C_1[v_x] + C_2[v_x] = -C_1[v_x]$, so that we finally obtain Eq. (55).

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