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Local density of states and scattering matrix in quasi-one-dimensional systems

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Mathematical relations between the local density of states (LDOS) and the scattering matrix (i.e., transmission and reflection amplitudes) for quasi-one-dimensional systems are derived in the presence of static uniform magnetic fields. Starting from the definition of the LDOS expressed by the Green's function, we derive the formulas for the LDOS in terms of the functional derivative of the scattering matrix or the Friedel phase with respect to a scattering potential.

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I. INTRODUCTION

The single-particle density of states (DOS) is one of the most important and useful concepts in the study of equilibrium thermodynamic properties of systems. Once the DOS is obtained, one can construct the thermodynamic potential from which any thermodynamic quantities can be derived.[1] Recently, the conceptual importance of DOS and its generalized version has been strongly emphasized in the study of mesoscopic physics.[2–4] It is well known that electronic transport phenomena in mesoscopic phase-coherent systems can be well described by Landauer-Büttiker scattering theoretical formalism.[5–7] Interestingly, the density of states and thus the thermodynamic quantities can be also described in the framework of the scattering theory as discussed in the following pioneering works: Dashen, Ma, and Burnstein[8] formulated equilibrium thermodynamics in terms of the scattering matrices, and Avishai and Band[9] presented the general relation between the scattering matrix and the global DOS in one-dimensional systems.

Subsequently, in the scattering theoretical formulation of ac transport, Büttiker and co-workers[10,11] generalized the concept of DOS by introducing the partial density of states and the local partial density of states (LPDOS), in which the use of scattering matrices is essential to extract *partial* contributions to the DOS. The information about the LPDOS is desirable for the description of ac or nonlinear transport states in order to take into account nonequilibrium charge distributions.[12–16] Also, the concept of the LPDOS is known to be essential to describe the dwell time of a particle in conductors.[17–19] Another example where the generalized DOS is important is the theory of tunneling current flowing through the scanning tunneling microscope tip.[20]

Although there is no doubt about the conceptual importance of those generalized densities of states, the problem of how to derive the scattering matrix representation of LDOS remains yet to be solved. Our main aim in this paper is to present a mathematical procedure to relate the local or global DOS to scattering matrices, starting from the well-known formula for DOS expressed by the Green's function.[1] For completeness of our discussion, the relation between the global density of states and the scattering matrix is also presented.

This paper is organized as follows. In the next section we present a brief description of the scattering problem in quasi-one-dimensional (Q1D) systems subjected to a static uniform magnetic field. Section III consists of six subsections. After introducing the definition of LDOS in the first subsection, we present in the second and third subsections the derivation of the relation between the potential-induced deviation of the global DOS (GDOS) and the scattering matrix, which is equivalent to the Friedel sum rule.[21–23] This part is the straightforward generalization of Avishai and Band's previous work[9] to the case of multichannel conductors subjected to a magnetic field. The fourth and fifth subsections are the central part of this paper, dealing with the problem of how the LDOS itself is expressed in terms of the scattering matrix. In the final subsection of Sec. III, we discuss the relation among the Friedel phase, GDOS, and LDOS. The summary of results and conclusions is presented in Sec. IV.

II. SCATTERING PROBLEM

In this section we briefly present a formal scattering theory of an electron in a Q1D system, which gives us an important mathematical basis to discuss the relationship between the density of states and the scattering matrix. To begin, let us consider a perfect Q1D wire with width W subjected to a static uniform perpendicular magnetic field. An electron in such a system is described by the Hamiltonian

$$H_0(\boldsymbol{r},\boldsymbol{p})=\frac{1}{2m}[\boldsymbol{p}-q\boldsymbol{A}(\boldsymbol{r})]^2+U(y), \tag{1}$$

where $\boldsymbol{p}=-i\hbar(\partial/\partial x,\partial/\partial y)$ is the momentum operator in a two-dimensional plane, $q=-|e|$ the charge of an electron with an effective mass m, and $\boldsymbol{A}(\boldsymbol{r})=-By\boldsymbol{e}_x$ the vector potential describing a static uniform magnetic field $\boldsymbol{B}=B\boldsymbol{e}_z$. The confinement potential $U(y)$ is zero for $|y|\leqslant W/2$ while it is ∞ otherwise (i.e., a hard-wall confinement potential). The eigenfunction of this free Hamiltonian H_0 can be expressed in the form separated in variables as

$$\Phi_{nk}^{\gamma(0)}(\boldsymbol{r})=\frac{1}{\sqrt{2\pi}}e^{\gamma ikx}\phi_{nk}^{\gamma}(y), \tag{2}$$

with the sign $\gamma=+(-)$ corresponding to the right (left) moving solution. Here $k\equiv|k|$ is the longitudinal wave number and $\phi_{nk}^{\gamma}(y)$ is the nth eigenfunction of the eigenvalue equation

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+\frac{m\omega_c^2}{2}[y-y_0(\gamma k)]^2+U(y)\right\}\phi_{nk}^{\gamma}(y)$$
$$=\varepsilon_n(k)\phi_{nk}^{\gamma}(y), \tag{3}$$

where $y_0(\gamma k)=\gamma l_B^2 k$ is the center of the cyclotron motion with $l_B=\sqrt{\hbar/(eB)}$ the magnetic length, and $\omega_{\rm c}=eB/m$ the cyclotron frequency. We assume that $\phi_{nk}^{\gamma}(y)$ is normalized such that $\int_{-W/2}^{W/2}dy|\phi_{nk}^{\gamma}(y)|^2=1$. Solving the eigenvalue Eq. (3) for a given wave number k, one can determine the single-particle energy $\varepsilon_n(k)$ (i.e., the eigenvalue of H_0) and the corresponding transverse wave function $\phi_{nk}^{\gamma}(y)$. In the absence of the confinement potential such that $U(y)=0$, Eq. (3) has eigenvalues $\varepsilon_n=(n+1/2)\hbar\omega_c$ (Landau levels) independent of the longitudinal wave number k and the center of cyclotron motion y_0. However the presence of the confinement potential $U(y)$ influences the cyclotron motion near the confinement walls (edges) of the conductor, giving rise to the formation of edge states. Then the energy eigenvalue ε_n depends on the longitudinal wave number k allowing electrons to have the longitudinal velocity $v_n(k)=(1/\hbar)\partial\varepsilon_n(k)/\partial k$. For a given electron energy E, we express the longitudinal wave number k satisfying the relation $E=\varepsilon_n(k)$ as $k_n(E)$ for each mode (subband) index n, and the longitudinal velocity $v_n[k=k_n(E)]$ as $v_n(E)$. Hereafter we shall write $k_n(E)$ and $v_n(E)$ simply as k_n and v_n, respectively. The free scattering state for a given energy E is then expressed as $\Phi_{nk_n(E)}^{\gamma(0)}(\boldsymbol{r})\equiv\Phi_{nk_n}^{\gamma(0)}(\boldsymbol{r})$.

Let us consider the case where the scattering potential $V(\boldsymbol{r})$ describing impurities or any static defects is present in addition to the free Hamiltonian $H_0(\boldsymbol{r},\boldsymbol{p})$: $H(\boldsymbol{r},\boldsymbol{p})=H_0(\boldsymbol{r},\boldsymbol{p})+V(\boldsymbol{r})$. We assume that the scattering potential $V(\boldsymbol{r})$ is restricted within a central finite region $\Omega=:\{|x|\leqslant L/2, |y|\leqslant W/2\}$. In the presence of the scattering potential $V(\boldsymbol{r})$, the free scattering state $\Phi_{nk_n}^{\gamma(0)}(\boldsymbol{r})$ evolves into the full scattering state $\Phi_{nk_n}^{\gamma}(\boldsymbol{r})$ which can be expressed by the Lippmann-Schwinger equation in terms of the retarded Green's function $G_0^R(\boldsymbol{r},\boldsymbol{r}',E)$ in the absence of scattering potential along with the T matrix $T(\boldsymbol{r},\boldsymbol{r}';E)$ given by $\hat{T}=\hat{V}+\hat{V}\hat{G}_0^R\hat{T}$ in operator form.[1] The full scattering state $\Phi_{nk_n}^{+}(\boldsymbol{r})$ at particular positions (x_R,y) in the right asymptotic region $(x_R\gg L/2)$ and (x_L,y) in the left asymptotic region $(x_L\ll -L/2)$ is readily expressed by

$$\Phi_{nk_n}^{+}(x_R,y)=\sum_{l=0}^{N_p}\Phi_{lk_l}^{+(0)}(x_R,y)\sqrt{\frac{|v_n|}{|v_l|}}\,s_{ln}^{++}(E), \tag{4}$$

$$\Phi_{nk_n}^{+}(x_L,y)=\Phi_{nk_n}^{+(0)}(x_L,y)$$
$$+\sum_{l=0}^{N_p}\Phi_{lk_l}^{-(0)}(x_L,y)\sqrt{\frac{|v_n|}{|v_l|}}\,s_{ln}^{-+}(E). \tag{5}$$

Here N_p denotes the largest mode index n satisfying the condition $\varepsilon_n(k=0)<E$ for which $k_n(E)$ and $v_n(E)$ are real numbers, and $s_{ln}^{\gamma\gamma'}(E)$ is given by

$$s_{ln}^{\gamma\gamma'}(E)=\delta_{ln}\delta_{\gamma\gamma'}+\frac{-i}{\hbar\sqrt{|v_l(E)v_n(E)|}}T_{lk_l,nk_n}^{\gamma\gamma'}(E), \tag{6}$$

where $T_{lk_l,nk_n}^{\gamma\gamma'}(E)$ $(\gamma,\gamma'=+,-)$ is the (lk_l,nk_n) element of the double Fourier-transformed T matrix given by

$$T_{lk_l,nk_n}^{\gamma\gamma'}(E)=\int d\boldsymbol{r}\int d\boldsymbol{r}'\,\Phi_{lk_l}^{\gamma(0)*}(\boldsymbol{r})T(\boldsymbol{r},\boldsymbol{r}';E)\Phi_{nk_n}^{\gamma'(0)}(\boldsymbol{r}'). \tag{7}$$

It is noted that Eq. (6) can be reduced to the Fisher-Lee relation[24] and the Baranger-Stone relation[25] in the absence and the presence of magnetic fields, respectively.

It is obvious from Eqs. (4) and (5) that s_{ln}^{++} (s_{ln}^{-+}) plays the role of the transmission (reflection) amplitude from the nth mode in the left asymptotic region to the lth mode in the right (left) asymptotic region. Similarly, the full scattering state $\Phi_{lk_l}^{-}(\boldsymbol{r})$ at those particular positions (x_L,y) and (x_R,y) can be expressed in terms of the transmission amplitude s_{ln}^{--} and the reflection amplitude s_{ln}^{+-}, respectively. Here s_{ln}^{--} (s_{ln}^{+-}) is interpreted as the transmission (reflection) amplitude from the right asymptotic region to the left (right) asymptotic region. Those transmission and reflection amplitudes s_{ln}^{++}, s_{ln}^{+-}, s_{ln}^{-+}, and s_{ln}^{--} compose a $2N_p\times 2N_p$ scattering matrix $\boldsymbol{S}(E)$:

$$\boldsymbol{S}(E)=\begin{pmatrix}\boldsymbol{s}^{++}(E) & \boldsymbol{s}^{+-}(E)\\ \boldsymbol{s}^{-+}(E) & \boldsymbol{s}^{--}(E)\end{pmatrix}, \tag{8}$$

where each submatrix $\boldsymbol{s}^{\gamma\gamma'}$ is a $N_p\times N_p$ matrix whose (l,n) element is the transmission or reflection amplitude $s_{ln}^{\gamma\gamma'}$ defined by Eq. (6). One can prove that the scattering matrix $\boldsymbol{S}$ is unitary owing to the Hermiticity of the scattering potential $V(\boldsymbol{r})$.

Before closing this section, we emphasize that the each scattering matrix element $s_{ln}^{\gamma\gamma'}$ is *not* associated with the phase evolution due to the free propagation of an electron. This is obvious from the fact that we have $s_{ln}^{\gamma\gamma'}=\delta_{ln}\delta_{\gamma\gamma'}$ in the case of $V(\boldsymbol{r})=0$. Therefore, in the presence of scattering potentials, the phase (argument) of the elements in the scattering matrix plays the role of transmission or reflection *phase shift* due to the presence of the scattering potential.

III. DENSITY OF STATES

In the previous section we have discussed the scattering problem of an electron in a Q1D system, and obtained the expression for the scattering matrix at a given energy E in terms of the T matrix. Our purpose in this section is to derive useful mathematical formulas for the density of states at a given energy E in terms of the scattering matrix at that energy.

A. Definition of the local density of states

In the case of open infinite systems such as a Q1D wire considered here, the density of states for an entire region becomes infinite because of the continuum energy spectrum of those systems. Thus what we should regard as a fundamental concept in such systems is the *local* density of states (LDOS). The LDOS at a particular position $\boldsymbol{r}$ for a given energy E is defined by using the full scattering wave function $\Phi^{\pm}_{nk}(\boldsymbol{r})$ as

$$\begin{aligned}\rho(\boldsymbol{r},E)&=\sum_{n=0}^{\infty}\sum_{\gamma=\pm}\int_0^{\infty}dk|\Phi^{\gamma}_{nk}(\boldsymbol{r})|^2\delta(E-\varepsilon_n(k))\\&=\frac{-1}{\pi}\,\mathrm{Im}\sum_{\gamma,n}\int_0^{\infty}dk\frac{\Phi^{\gamma}_{nk}(\boldsymbol{r})\Phi^{\gamma *}_{nk}(\boldsymbol{r})}{E-\varepsilon_n(k)+i0_+}\\&=\frac{-1}{\pi}\,\mathrm{Im}\,G^R(\boldsymbol{r},\boldsymbol{r};E),\end{aligned}\tag{9}$$

where we have used the formula $1/(x+i0_+)=\mathrm{P}(1/x)-i\pi\delta(x)$. Here $G^R(\boldsymbol{r},\boldsymbol{r};E)$ is the diagonal elements of the retarded Green's function which satisfies

$$[E-H(\boldsymbol{r},\boldsymbol{p})+i0_+]G^R(\boldsymbol{r},\boldsymbol{r}';E)=\delta(\boldsymbol{r}-\boldsymbol{r}').\tag{10}$$

Corresponding to the fact that the total Hamiltonian is given by $H(\boldsymbol{r},\boldsymbol{p})=H_0(\boldsymbol{r},\boldsymbol{p})+V(\boldsymbol{r})$, the retarded Green's function follows the Dyson-type equation

$$\begin{aligned}G^R(\boldsymbol{r},\boldsymbol{r}';E)=G^R_0(\boldsymbol{r},\boldsymbol{r}';E)+\int d\boldsymbol{r}_1\int d\boldsymbol{r}_2G^R_0(\boldsymbol{r},\boldsymbol{r}_1;E)\\\times T(\boldsymbol{r}_1,\boldsymbol{r}_2;E)G^R_0(\boldsymbol{r}_2,\boldsymbol{r}';E),\end{aligned}\tag{11}$$

where $G^R_0(\boldsymbol{r},\boldsymbol{r}';E)$ is the retarded Green's function for the *free* Hamiltonian H_0 and $T(\boldsymbol{r},\boldsymbol{r}';E)$ denotes the T matrix. A set of Eqs. (9) and (11) is the starting point in our subsequent discussions.

B. Deviation of the global density of states due to scattering potential

Although the LDOS itself is an important concept, it is also useful to know how the presence of scattering potential influences the DOS for an entire region. From now on, the DOS for an entire region is referred to as the *global* density of states (GDOS). If we substitute Eq. (11) into Eq. (9), the LDOS $\rho(\boldsymbol{r},E)$ can be expressed as a sum of two terms:

$$\rho(\boldsymbol{r},E)=\rho_0(\boldsymbol{r},E)+\Delta\rho(\boldsymbol{r},E),\tag{12}$$

$$\rho_0(\boldsymbol{r},E)\equiv\sum_{n=1}^{N_p}\frac{1}{\pi\hbar v_n(E)}\sum_{\gamma=\pm}|\phi^{\gamma}_{nk(E)}(y)|^2,\tag{13}$$

$$\Delta\rho(\boldsymbol{r},E)\equiv-\frac{1}{\pi}\,\mathrm{Im}\langle\boldsymbol{r}|\hat{G}^R_0(E)\hat{T}(E)\hat{G}^R_0(E)|\boldsymbol{r}\rangle,\tag{14}$$

where $\hat{G}^R_0(E)$ and $\hat{T}(E)$ are operators corresponding to the retarded Green's function and the T matrix, respectively. In Eq. (12), $\rho_0(\boldsymbol{r},E)\equiv\rho_0(x,y;E)$ is the LDOS in the absence of the scattering potential, and is independent of the longitudinal coordinate x, while $\Delta\rho(\boldsymbol{r},E)\equiv\Delta\rho(x,y;E)$ is the deviation of the LDOS due to the presence of the scattering potential. In the absence of scattering potentials, the fact $T(\boldsymbol{r},\boldsymbol{r}';E)=0$ ensures the expected result, viz., $\rho(\boldsymbol{r},E)=\rho_0(\boldsymbol{r},E)$. In the presence of scattering potentials, however, the quantity $\Delta\rho(\boldsymbol{r},E)$ is integrated spatially over an entire region yielding

$$\begin{aligned}\Delta D(E)&\equiv\int_{-\infty}^{\infty}dx\int_{-W/2}^{W/2}dy\,\Delta\rho(x,y,E)\\&=-\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}\{\hat{G}^R_0(E)\hat{T}(E)\hat{G}^R_0(E)\}.\end{aligned}\tag{15}$$

Evaluation of this equation gives us the information on how the presence of scattering potential $V(\boldsymbol{r})$ influences the GDOS at a given energy E. As shown in the detailed calculation given in Appendix A, Eq. (15) can be expressed in a simple form:

$$\Delta D(E)=\frac{1}{2\pi i}\frac{\partial}{\partial E}\,\mathrm{Tr}\{\ln\hat{S}(E)\},\tag{16}$$

with

$$\hat{S}(E)\equiv\hat{I}-2\pi i\,\delta(E\hat{I}-\hat{H}_0)\hat{T}(E)\tag{17}$$

the scattering operator. In Eq. (16), we introduced the logarithmic operator function by applying the formula $\ln(\hat{I}-\hat{A})=-\Sigma_{n=1}^{\infty}(\hat{A}^n/n)$, where $\hat{A}$ is an arbitrary operator. Equation (16) is an exact relation connecting a given functional form of the scattering potential $V(\boldsymbol{r})$ and the change of GDOS due to the presence of scattering potential. In order to compare the quantity $\Delta D(E)$ to the scattering matrix $\boldsymbol{S}$ (and hence the transmission and reflection amplitudes), we need to evaluate the trace of the operator $\ln\hat{S}$. To do this, let us define an operator $\hat{X}(E)\equiv 2\pi i\,\delta(E-\hat{H}_0)\hat{T}(E)$. Then, what we need to evaluate is the quantity $\mathrm{Tr}\{\ln\hat{S}\}=\mathrm{Tr}\{\ln(\hat{I}-\hat{X})\}=-\Sigma_{m=1}^{\infty}(\mathrm{Tr}\{\hat{X}^m\}/m)$. The trace of the mth power of the operator $\hat{X}$ is calculated as

$$\begin{aligned}\mathrm{Tr}\{[\hat{X}(E)]^m\}&=\sum_{n=0}^{\infty}\sum_{\gamma=\pm}\int_0^{\infty}dk\langle\Phi^{\gamma(0)}_{n,k}|[\hat{X}(E)]^m|\Phi^{\gamma(0)}_{n,k}\rangle\\&=\sum_{n=0}^{N_p}\sum_{\gamma=\pm}\{[\boldsymbol{X}(E)]^m\}_{\gamma n,\gamma n}=:\mathrm{tr}\{[\boldsymbol{X}(E)]^m\},\end{aligned}\tag{18}$$

where $\boldsymbol{X}(E)$ is a $2N_p\times 2N_p$ matrix and its elements are given by

$$\{\boldsymbol{X}(E)\}_{\gamma l,\gamma' n}=\frac{-i}{\hbar\sqrt{v_l(E)v_n(E)}}T^{\gamma\gamma'}_{lk_l(E),nk_n(E)}(E),$$

$$(\gamma,\gamma'=\pm,\quad n,l=1,\ldots,N_p),\tag{19}$$

with $T^{\gamma\gamma'}_{l,k_l(E);n,k_n(E)}(E)$ given by Eq. (7). In Eq. (18), the trace symbol $\mathrm{tr}\{\cdots\}$ denotes the trace over $2N_p$ propagating channels, and was introduced to distinguish it from the trace symbol Tr which is used to trace an operator over a complete set of the Hilbert space. Substituting Eqs. (18) and (19) into Eq. (16), we finally arrive at important results:

$$\Delta D(E)=\frac{1}{2\pi i}\frac{d}{dE}\,\mathrm{tr}\{\ln \boldsymbol{S}(E)\} \tag{20a}$$

$$=\frac{1}{2\pi i}\,\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}(E)\frac{d\boldsymbol{S}(E)}{dE}\right\} \tag{20b}$$

$$=\frac{1}{4\pi i}\,\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}(E)\frac{d\boldsymbol{S}(E)}{dE}-\mathrm{H.c.}\right\}. \tag{20c}$$

Here $\boldsymbol{S}(E)=\boldsymbol{I}-\boldsymbol{X}(E)$ is the scattering matrix defined by Eq. (8). To obtain these results, the unitarity of the scattering matrix ($\boldsymbol{S}^{-1}=\boldsymbol{S}^{\dagger}$) has been used several times. In deriving Eq. (20c) from Eq. (20b), we used the fact that the unitarity of the scattering matrix ensures that the quantity $\mathrm{tr}\{\boldsymbol{S}^{\dagger}(d/dE)\boldsymbol{S}\}$ is a pure imaginary number (see Appendix B). Equations (20a)–(20c) are desired relations relating $\Delta D(E)$ to the transmission and reflection amplitudes. Owing to the unitarity of $\boldsymbol{S}$, one can further rewrite Eqs. (20a)–(20c) in the form

$$\Delta D(E)=\frac{1}{\pi}\frac{\partial}{\partial E}\theta_F(E), \tag{21}$$

$$\theta_F(E)\equiv\frac{1}{2i}\ln[\det \boldsymbol{S}(E)], \tag{22}$$

where θ_F is called the Friedel phase.[21] That is, the deviation of the global density of states caused by a scattering potential $V(\boldsymbol{r})$ is *directly* related to the energy derivative of the Friedel phase. Recently, the relation Eq. (22) played an important role in the study of the transmission phase in mesoscopic systems.[26–28]

C. Decomposition of $\Delta D(E)$ into partial contributions

Recalling that the scattering matrix $\boldsymbol{S}$ can be decomposed into four submatrices $\boldsymbol{s}^{\gamma\gamma'}$ [see Eq. (8)], the quantity $\Delta D(E)$ expressed by Eq. (20c) can be rewritten as a sum of four terms:

$$\Delta D(E)=\sum_{\gamma,\gamma'=\pm}\Delta D^{\gamma\gamma'}(E), \tag{23}$$

$$\Delta D^{\gamma\gamma'}(E)\equiv\frac{1}{2\pi i}\,\mathrm{tr}\left\{(\boldsymbol{s}^{\gamma\gamma'})^{\dagger}\frac{d}{dE}\boldsymbol{s}^{\gamma\gamma'}-\mathrm{H.c.}\right\}. \tag{24}$$

In Eq. (24), the quantity $\Delta D^{++}(E)$ $[\Delta D^{-+}(E)]$ includes the transmission (reflection) amplitude matrix $\boldsymbol{s}^{++}$ $(\boldsymbol{s}^{-+})$. Thus, $\Delta D^{++}(E)$ $[\Delta D^{-+}(E)]$ is naturally interpreted as a partial contribution to $\Delta D(E)$ due to those electrons incoming from the left asymptotic region and transmitted (reflected) into the right (left) asymptotic region. Similarly, the quantity $\Delta D^{--}(E)$ $[\Delta D^{+-}(E)]$ is interpreted as a partial contribution to $\Delta D(E)$ due to those electrons incoming from the right asymptotic region and transmitted (reflected) into the left (right) asymptotic region. It should be noted that the quantity $\Delta D^{\gamma\gamma'}(E)$ given by Eq. (24) is certainly a real number.

D. Relation between the LDOS and the scattering matrix

Having understood that the deviation of the LDOS caused by a scattering potential is integrated spatially over a whole region to yield the energy derivative of the Friedel phase, our next question is how the local density of states at a particular position can be expressed in terms of the Friedel phase or the transmission/reflection amplitudes. As seen in Eq. (9), the LDOS itself can be expressed in terms of the Green's function as

$$\rho(\boldsymbol{r};E,\{\hat{V}\})=-\frac{1}{\pi}\,\mathrm{Im}\,G^R(\boldsymbol{r},\boldsymbol{r};E,\{\hat{V}\}), \tag{25}$$

where $\{\hat{V}\}$ denotes the functional form of the scattering potential $V(\boldsymbol{r})$. It should be noted that the Green's function and hence the LDOS are in general expressed by the functional of the scattering potential $V(\boldsymbol{r})$.

In order to relate this expression to the scattering matrix, let us first express the Green's function in the form perturbatively expanded with respect to the scattering potential $V(\boldsymbol{r})$ as

$$G^R(\boldsymbol{r},\boldsymbol{r}';E,\{\hat{V}\})=\langle\boldsymbol{r}|\hat{G}^R_0(E)\sum_{n=0}^{\infty}(\hat{V}\hat{G}^R_0(E))^n|\boldsymbol{r}'\rangle. \tag{26}$$

As a next step, we introduce the following functional:

$$F(E,\{\hat{V}\})\equiv\int d\boldsymbol{r}\int d\boldsymbol{r}_1 G^R_0(\boldsymbol{r},\boldsymbol{r}_1;E)T(\boldsymbol{r}_1,\boldsymbol{r};E,\{\hat{V}\})$$
$$=\mathrm{Tr}\{\hat{G}^R_0(E)\hat{T}(E,\{\hat{V}\})\}. \tag{27}$$

By substituting the T matrix into this equation iteratively, the functional $F(E,\{\hat{V}\})$ can be expressed in terms of $\hat{G}^R_0(E)$ as a summation over an infinite number of terms:

$$F(E,\{\hat{V}\})=\sum_{n=1}^{\infty}F_n(E,\{\hat{V}\}), \tag{28}$$

$$F_n(E,\{\hat{V}\})=\mathrm{Tr}\{(\hat{G}^R_0(E)\hat{V})^n\}. \tag{29}$$

We note that the nth functional $F_n(E,\{\hat{V}\})$ corresponds to the nth-order term with respect to the scattering potential $V(\boldsymbol{r})$. To proceed further, let us consider the functional derivative of F_n with respect to the scattering potential $V(\boldsymbol{r})$, which is defined by

$$\frac{\delta F_n(E,\{\hat{V}\})}{\delta V(\boldsymbol{r}_1)}\equiv\lim_{\epsilon\to 0}\frac{1}{\epsilon}[F_n(E,\{\hat{V}+\epsilon\hat{\delta}_{\boldsymbol{r}_1}\})-F_n(E,\{\hat{V}\})]. \tag{30}$$

Here $\epsilon\hat{\delta}_{\boldsymbol{r}_1}$ represents the functional form of the scattering potential $\epsilon\delta(\boldsymbol{r}-\boldsymbol{r}_1)$ which is localized at a particular position $\boldsymbol{r}_1$. We note that the quantity ϵ should have the dimension of [energy×length], meaning that the dimension of the functional derivative $\delta F_n(E,\{\hat{V}\})/\delta V(\boldsymbol{r}_1)$ is [1/(energy×length)] in contrast to the energy derivative $\partial F_n(E,\{\hat{V}\})/\partial E$ which has the dimension of [1/energy]. By substituting Eq. (29) into Eq. (30), we obtain the functional derivative of the functional F_n as

$$\frac{\delta F_n(E,\{\hat{V}\})}{\delta V(\boldsymbol{r})}=n\langle \boldsymbol{r}|\hat{G}_0^R(E)[\hat{V}\hat{G}_0^R(E)]^{n-1}|\boldsymbol{r}\rangle. \tag{31}$$

Comparing this equation with the Green's function Eq. (26), diagonal elements of the retarded Green's function can be expressed in terms of the functional $F_n(E,\{\hat{V}\})$ as

$$G^R(\boldsymbol{r},\boldsymbol{r};E,\{\hat{V}\})=\sum_{n=1}^{\infty}\frac{1}{n}\frac{\delta F_n(E,\{\hat{V}\})}{\delta V(\boldsymbol{r})}. \tag{32}$$

If we rewrite this equation by using the expression for F_n given by Eq. (29), we arrive at an important equation:

$$\begin{aligned}G^R(\boldsymbol{r},\boldsymbol{r};E,\{\hat{V}\})&=\frac{-\delta}{\delta V(\boldsymbol{r})}\,\mathrm{Tr}\left\{\sum_{n=1}^{\infty}\frac{-1}{n}(\hat{G}_0^R(E)\hat{V})^n\right\}\\&=\frac{-\delta}{\delta V(\boldsymbol{r})}\,\mathrm{Tr}\{\ln(\hat{I}-\hat{G}_0^R(E)\hat{V})\}.\end{aligned} \tag{33}$$

Taking the imaginary part of this equation with the help of Eq. (A3) in Appendix A and substituting it into Eq. (25), we finally obtain

$$\rho(\boldsymbol{r};E,\{\hat{V}\})=\frac{-1}{2\pi i}\frac{\delta}{\delta V(\boldsymbol{r})}\,\mathrm{Tr}\{\ln\hat{S}(E,\{\hat{V}\})\}, \tag{34}$$

with $\hat{S}$ the scattering operator given by Eq. (17). In the same procedure as used to obtain Eqs. (20a)–(20c), the trace over the complete set of the Hilbert space in Eq. (34) is carried out, yielding

$$\rho(\boldsymbol{r};E,\{\hat{V}\})=\frac{-1}{2\pi i}\frac{\delta}{\delta V(\boldsymbol{r})}\,\mathrm{tr}\{\ln\boldsymbol{S}(E,\{\hat{V}\})\} \tag{35a}$$

$$=\frac{-1}{2\pi i}\,\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}\frac{\delta\boldsymbol{S}}{\delta V(\boldsymbol{r})}\right\} \tag{35b}$$

$$=\frac{-1}{4\pi i}\,\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}\frac{\delta\boldsymbol{S}}{\delta V(\boldsymbol{r})}-\mathrm{H.c.}\right\}. \tag{35c}$$

The LDOS can be expressed in terms of the unitary scattering matrix (i.e., transmission and reflection amplitudes) defined by Eq. (8). The trace symbol tr in Eqs. (35a)–(35c) denotes the trace over $2N_p$ propagating modes. Equivalently, the LDOS can be expressed in terms of the Friedel phase defined by Eq. (22) as

$$\rho(\boldsymbol{r};E,\{\hat{V}\})=-\frac{1}{\pi}\frac{\delta}{\delta V(\boldsymbol{r})}\theta_F(E,\{\hat{V}\}). \tag{36}$$

That is, the LDOS at a particular position $\boldsymbol{r}$ for those electrons having an energy E can be evaluated from the functional derivative of the Friedel phase at that energy E with respect to the scattering potential $V(\boldsymbol{r})$. The results [Eqs. (35a)–(35c)] obtained here are very similar to Eqs. (20a)–(20c), respectively. Here the energy derivative of the scattering matrix or the Friedel phase is replaced by the functional derivative with respect to the scattering potential.

E. Local partial density of states

In Eqs. (35b) and (35c), the LDOS is expressed in terms of the unitary scattering matrix $\boldsymbol{S}$. Therefore, one can rewrite the LDOS in terms of the transmission or reflection amplitude submatrices. By substituting Eq. (8) into Eq. (35c), the LDOS is expressed as a sum of partial contributions:

$$\rho(\boldsymbol{r};E,\{\hat{V}\})=\sum_{\gamma,\gamma'=\pm}\rho^{\gamma\gamma'}(\boldsymbol{r};E,\{\hat{V}\}), \tag{37}$$

where

$$\rho^{\gamma\gamma'}(\boldsymbol{r};E,\{\hat{V}\})=\frac{-1}{4\pi i}\,\mathrm{tr}\left\{(\boldsymbol{s}^{\gamma\gamma'})^{\dagger}\frac{\delta\boldsymbol{s}^{\gamma\gamma'}}{\delta V(\boldsymbol{r})}-\mathrm{H.c.}\right\} \tag{38}$$

is called the local partial density of states (LPDOS) since it is a partial contribution to the LDOS (see below). It should be noted that the LPDOS given by Eq. (38) is a real quantity. Physical meaning of the LPDOS is as follows. For instance, $\rho^{++}(\boldsymbol{r},E)$ $[\rho^{-+}(\boldsymbol{r},E)]$ describes the LPDOS at a particular position $\boldsymbol{r}$ due to those electrons incoming from the left asymptotic region and transmitted (reflected) into the right (left) asymptotic region. Another LPDOS $\rho^{--}(\boldsymbol{r},E)$ $[\rho^{+-}(\boldsymbol{r},E)]$ is also interpreted in the same manner for electrons incoming from the right asymptotic region. In recent literature,[2,3] a quantity $\Sigma_{\gamma=\pm}\rho^{\gamma+}(\boldsymbol{r};E)$ $[\Sigma_{\gamma=\pm}\rho^{\gamma-}(\boldsymbol{r};E)]$ is called the *injectivity* for those electrons injected from the left (right) asymptotic region. On the other hand, $\Sigma_{\gamma=\pm}\rho^{+\gamma}(\boldsymbol{r};E)$ $[\Sigma_{\gamma=\pm}\rho^{-\gamma}(\boldsymbol{r};E)]$ is called the *emissivity* for those electrons emitted into the right (left) asymptotic regions. Injectivity and emissivity play important roles in the theory of ac and nonlinear transport in mesoscopic conductors to describe the response due to local charge distributions.[2–4,10–16]

F. Role of the Friedel phase in the density of states

Finally we consider the relationship between the energy derivative of the Friedel phase and the functional derivative of the Friedel phase with respect to the scattering potential. For this purpose, we write $\Delta D(E)$ from Eqs. (12) and (15) as

$$\Delta D(E)=\int d\boldsymbol{r}(\rho(\boldsymbol{r};E,\{\hat{V}\})-\rho_0(\boldsymbol{r},E)), \tag{39}$$

where $\rho_0(\boldsymbol{r},E)$ is the LDOS in the absence of the scattering potential. Noting that the quantity $\Delta D(E)$ and the LDOS $\rho(\boldsymbol{r},E)$ have been expressed in terms of the Friedel phase

[Eq. (22)] as seen in Eq. (21) and Eq. (36), both sides of Eq. (39) can be rewritten using the Friedel phase as

$$-\frac{\partial}{\partial E}\theta_F(E)=\int d\boldsymbol{r}\frac{\delta}{\delta V(\boldsymbol{r})}[\theta_F(E,\{\hat{V}\})-\theta_F^{(1)}(E,\{\hat{V}\})], \tag{40}$$

where

$$\theta_F^{(1)}(E,\{\hat{V}\})=-\pi\int d\boldsymbol{r}\rho_0(\boldsymbol{r},E)V(\boldsymbol{r}) \tag{41}$$

is the first-order term in the functional expansion of the Friedel phase with respect to the scattering potential $V(\boldsymbol{r})$. We note that the zeroth-order term of the Friedel phase with respect to $V(\boldsymbol{r})$ is given by $\theta_F^{(0)}(E,\{\hat{V}\})=\theta_F(E,\{\hat{V}=0\})$, which can be chosen as 0 independent of the energy since the scattering matrix in Eq. (8) does not include the phase evolution due to free propagations of electrons. Equation (40) is an important relation connecting the energy derivative of the Friedel phase to the functional derivative of the Friedel phase with respect to the scattering potential.

IV. CONCLUSION

In conclusion, we have investigated the mathematical relationship between the LDOS and the scattering matrix for quasi-one-dimensional systems in the presence of static perpendicular magnetic fields. Starting from the definition of LDOS in terms of the Green's function, we derived the scattering matrix representation of the LDOS in a straightforward way. While the scattering potential-induced deviation of the GDOS is expressed in terms of the energy derivative of the scattering matrix, the LDOS itself is expressed in terms of the functional derivative of the scattering matrix with respect to the scattering potential. Alternately, the potential-induced deviation of the GDOS and the LDOS are also expressed in terms of the energy derivative of the Friedel phase and the functional derivative of the Friedel phase with respect to the scattering potential, respectively. Finally, we derived the relation between the energy derivative of the Friedel phase and the functional derivative of the Friedel phase with respect to the scattering potential. Although our discussion is concentrated on the densities of states in narrow two-dimensional (2D quantum waveguide) systems, our theory can be generalized to three-dimensional quantum waveguide (tube) systems straightforwardly.

APPENDIX A: DERIVATION OF EQ. (16)

In this appendix we present the derivation of Eq. (16). In Eq. (18), the operator Green's function is expressed as $\hat{G}^R(E)=((E+i0_+)\hat{I}-\hat{H})^{-1}$. Thus the trace in Eq. (15) can be expressed by

$$\begin{aligned}&\mathrm{Tr}\{\hat{G}_0^R(E)\hat{T}(E)\hat{G}_0^R(E)\}\\&\quad=\mathrm{Tr}\{\hat{G}_0^R(E)\hat{G}_0^R(E)\hat{T}(E)\}=\mathrm{Tr}\left[-\frac{d\hat{G}_0^R(E)}{dE}\hat{T}(E)\right].\end{aligned} \tag{A1}$$

Let us substitute this expression into Eq. (15). Since the T operator is expressed as $\hat{T}=\hat{V}\Sigma_{n=0}^{\infty}[\hat{G}_0^R(E)\hat{V}]^n$, $\Delta D(E)$ is calculated as

$$\begin{aligned}\Delta D(E)&=-\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}\left\{\left[-\frac{\partial\hat{G}_0^R(E)}{\partial E}\right]\hat{T}(E)\right\}\\&=-\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}\left\{-\frac{\partial\hat{G}_0^R(E)}{\partial E}\hat{V}\sum_{n=0}^{\infty}[\hat{G}_0^R(E)\hat{V}]^n\right\}\\&=-\frac{1}{\pi}\,\mathrm{Im}\sum_{n=1}^{\infty}\frac{-1}{n}\,\mathrm{Tr}\left\{\frac{\partial}{\partial E}[\hat{G}_0^R(E)\hat{V}]^n\right\}\\&=-\frac{1}{\pi}\,\mathrm{Im}\,\frac{\partial}{\partial E}\,\mathrm{Tr}\left\{\sum_{n=1}^{\infty}\frac{-1}{n}[\hat{G}_0^R(E)\hat{V}]^n\right\}\\&=-\frac{1}{\pi}\,\mathrm{Im}\,\frac{\partial}{\partial E}\,\mathrm{Tr}\{\ln[\hat{I}-\hat{G}_0^R(E)\hat{V}]\}.\end{aligned} \tag{A2}$$

The right-hand side of this equation can be further simplified by the following procedure:

$$\begin{aligned}&-\mathrm{Im}\,\mathrm{Tr}\{\ln[\hat{I}-\hat{G}_0^R(E)\hat{V}]\}\\&\quad=-\frac{1}{2i}[\mathrm{Tr}\{\ln(\hat{I}-\hat{G}_0^R(E)\hat{V}t)\}-\mathrm{c.c}]\\&\quad=\frac{1}{2i}\,\mathrm{Tr}\{\ln[(\hat{I}-\hat{G}_0^A(E)\hat{V})(\hat{I}-\hat{G}_0^R(E)\hat{V})^{-1}]\}\\&\quad=\frac{1}{2i}\,\mathrm{Tr}\{\ln[\hat{I}-\{\hat{G}_0^A(E)-\hat{G}_0^R(E)\}\hat{T}(E)]\}\\&\quad=\frac{1}{2i}\,\mathrm{Tr}\{\ln[\hat{I}-2\pi i\,\delta(E-\hat{H}_0)\hat{T}(E)]\}\\&\quad=\frac{1}{2i}\,\mathrm{Tr}\{\ln\hat{S}(E)\},\end{aligned} \tag{A3}$$

where $\hat{S}(E)\equiv\hat{I}-2\pi i\,\delta(E-\hat{H}_0)$ is the scattering operator. Substituting this result into Eq. (A2), we obtain Eq. (16).

APPENDIX B:

The purpose of this appendix is to show that the quantity $\mathrm{tr}\{\boldsymbol{S}^{\dagger}(E)(d/dE)\boldsymbol{S}(E)\}$ in Eq. (20b) is a pure imaginary number. Let us start from the fact that the $2N_p\times 2N_p$ scattering matrix given by Eq. (8) is unitary such that

$$\boldsymbol{S}^{\dagger}(E)\boldsymbol{S}(E)=\boldsymbol{I}. \tag{B1}$$

Differentiating Eq. (B1) with respect to energy and taking the trace over $2N_p$ propagating channels, we obtain

$$\mathrm{tr}\left\{\left[\frac{d}{dE}\boldsymbol{S}^{\dagger}(E)\right]\boldsymbol{S}(E)\right\}+\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}(E)\frac{d}{dE}\boldsymbol{S}(E)\right\}=0. \tag{B2}$$

Here the complex conjugate of the second term in the left-hand side becomes

$$\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}(E)\frac{d}{dE}\boldsymbol{S}(E)\right\}^{*}=\mathrm{tr}\left\{\left[\frac{d}{dE}\boldsymbol{S}^{\dagger}(E)\right]\boldsymbol{S}(E)\right\}. \tag{B3}$$

Thus Eq. (B2) is rewritten as

$$\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}(E)\frac{d}{dE}\boldsymbol{S}(E)\right\}^{*}=-\mathrm{tr}\left\{\boldsymbol{S}^{\dagger}(E)\frac{d}{dE}\boldsymbol{S}(E)\right\}, \tag{B4}$$

meaning that the quantity $\mathrm{tr}\{\boldsymbol{S}^{\dagger}(E)(d/dE)\boldsymbol{S}(E)\}$ is a *pure imaginary*. Therefore one can conclude that the right-hand side of Eq. (20b) is certainly a *real* number as expected. By using the similar procedure, one can show that the right-hand side of Eq. (35b) is also a real number.

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