THE NEW METHOD OF THE THERMOMAGNETIC CURRENT CALCULATION. QUANTUM WIRE

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The method of the effective Hamiltonian (MEH) is offered for the calculation of the non-dissipative thermomagnetic current in the quantum wire. This method includes the temperature in the Hamiltonian as opposed to the previous researches. The calculation is done in the coherent-state representation for the parabolic quantum wire and non-degenerate statistics.

Calculated by the instrumentality of MEH the non-diagonal component of the thermomagnetic tensor is in full accord with results obtained previously. It should be noted that MEH needs no account of the electron diamagnetism.

In the presence of an electric field $\vec{E}$, a temperature gradient ∇T and a magnetic field $\vec{H}$, the current density has the form

$$j_i = \sigma_{ik} E_k - \beta_{ik} \nabla_k T \tag{1}$$

Here σ_{ik} and β_{ik} are the components of the conductivity tensors. The non-dissipative component of the thermomagnetic tensor β_{yx} was calculated by many authors [1]. But in those papers the temperature was not included in the Hamiltonian because the temperature is related to the statistical force.

The method including the temperature in the Hamiltonian was offered in [2] for a bulk sample. The paper [2] deals with the calculation of the thermomagnetic current based on the assumption that the presence of a temperature gradient in the system is analogous to an effect of a certain effective external electric field. This is one more method of calculating the thermomagnetic current based on the introduction of an effective Hamiltonian. As distinct from [2] the purpose of the present paper is using given method for the one of the nanoelectronics main object, the quantum wire (see for example [3]).

All the calculation in this paper are made in the basis of coherent states.

Let the sample of the crystal wherein the external strong magnetic field $\vec{H}$ is directed along the z axis be limited by the planes $x = x_i = -\frac{1}{2}L_x$ and $x = x_f = \frac{1}{2}L_x$, $y_i = -\frac{1}{2}L_y$ and $y_f = \frac{1}{2}L_y$, $z_i = -\frac{1}{2}L_z$ and $z_f = \frac{1}{2}L_z$. The sample is placed in a thermostat so that for all the points of the space with $x \le -\frac{1}{2}L_x$ the temperature is kept constant and equal to $T=T_0=const$, and for all the points of the space with $x \ge \frac{1}{2}L_x$ $T=T_f=const$. The temperature gradient in the sample is directed along the x axis, i.e. $T=T(x)$ for all points satisfying the inequality $-\frac{1}{2}L_x < x < \frac{1}{2}L_x$.

Let as suppose that we have to deal with a weakly non-uniform system. Then the temperature deviation from its equilibrium magnitude is small, say, in the simplest case of constant temperature gradient

$$T(x) = T_0\left[1 + \delta\left(xL_x^{-1} + \frac{1}{2}\right)\right] \tag{2}$$

where $\delta << 1$.

By assumption $T=T(x)$ and does not depend on y or z. Then in the absence of the external electric field (electrostatic potential $\varphi=0$) and the chemical potential $\xi=const$ we derive from (1) and (2)

$$j_y = -\beta_{yx}\frac{\partial T(x)}{\partial x} = -\beta_{yx}\frac{\delta T_0}{L_x} \tag{3}$$

We calculate this current, starting from the well know expression

$$j_y = -enTr\hat{\rho}\hat{v}_y \tag{4}$$

where ($-e$) is the electron charge, n is the density of conductivity electrons, $\hat{\rho}$ is the non-equilibrium electron density matrix:

$$\hat{\rho} = Z^{-1}\exp\left[-(\hat{H} - \xi)/kT\right] \tag{5}$$

Here Z is the partition function and k is Boltzmann's constant. In the expression

$$\frac{1}{T} = \left[1 - \delta\left(\frac{x}{L_x} + \frac{1}{2}\right)\right]\frac{1}{T_0} \tag{6}$$

is expanded in $\delta<<1$. Henceforth we restrict ourselves to the first-order terms in δ

$$\hat{H} = \hat{H}_0 - k\vec{r}\,gradT\,. \tag{7}$$

The second term in equation (7) is connected with the inclusion of the temperature gradient effect on the Hamiltonian of the equilibrium system $\hat{H}_0$. By analogy with the electric field, we assume that the temperature is the potential of a certain external field with the intensity, – grad T. The corresponding potential energy takes the form, $-k\vec{r}\cdot gradT$, with in the case under consideration is reduced to $-k\delta T_0/L_x$. Consequently, in constructing the Hamiltonian

(7) we proceed from the formal correspondence of the electrostatic potential φ with temperature T and the absolute value of the electron charge e with Boltzmann constant k.

Finally, instead of equation (5) we obtain

$$\hat{\rho} = Z^{-1} exp(-\hat{H}\gamma) \quad (8)$$

where

$$\gamma = (kT_0)^{-1}, \qquad \hat{H} = \hat{H}_0 - \xi + \hat{V} \quad (9)$$

$$\hat{V} = \delta\xi\left(\frac{x}{L_x} + \frac{1}{2}\right) - \frac{\delta}{\gamma}\frac{x}{L_x} - \frac{\delta}{2}\left(\hat{H}_0\frac{x}{L_x} + \frac{x}{L_x}\hat{H}_0 + \hat{H}_0\right) \quad (10)$$

The Hermiticity of the operator $\hat{V}$ is realized by the symmetrization of the product of the operators $\hat{H}_0$ and x.

From equation (8) one can see that in the presence of a small and uniform temperature gradient the density matrix of the system is similar to that of this same system in the absence of the temperature gradient, but exposed to an external field whose contribution to the Hamiltonian of the system is given by the operator $\hat{V}$. It is clear from (10) that $\hat{V}$ is a small perturbation, as it is proportional to the parameter of smallness δ. Hence, we expand the density matrix (8) in a series using perturbation theory and restrict ourselves to a linear approximation of the parameter of smallness:

$$\hat{\rho} = \hat{\rho}_0 + \hat{\rho}_1 \quad (11)$$

where the equilibrium matrix is given by

$$\hat{\rho}_0 = Z^{-1} exp\left[-(\hat{H}_0 - \xi)\gamma\right] \quad (12)$$

and the non-equilibrium addition to the density matrix is

$$\hat{\rho}_1 = -\hat{\rho}_0\int_0^{\gamma} d\gamma' exp(\hat{H}_0\gamma')\hat{V} exp(-\hat{H}_0\gamma') \quad (13)$$

Starting from the well known expression for the velocity operator

$$\hat{v}_y = (i/\hbar)\left[\hat{H}, y\right] \quad (14)$$

we write equation (4) to first order in δ:

$$j_y = -(ien/\hbar)Tr\left(\hat{\rho}_0\left[\hat{H}_0, y\right] + \hat{\rho}_0\left[\hat{V}, y\right] + \hat{\rho}_1\left[\hat{H}_0, y\right]\right) \quad (15)$$

In present paper $\hat{H}_0$ is

$$\hat{H}_0 = \frac{1}{2m}\left[\hat{p}_x^2 + (\hat{p}_y + m\omega_c x)^2 + \hat{p}_x^2\right] + \frac{m\omega_0^2(x^2 + z^2)}{2} \quad (16)$$

i.e. we consider a parabolic quantum wire (QW) in a quantizing magnetic field $\vec{H} \parallel z$, and vector potential $\vec{A} = (0, Hx, 0)$. The QW is directed along the y axis, ω_0 characterizes the parabolic potential of the QW, $\omega_c = eH/mc$ is the cyclotron frequency.

The coherent states (CS) for the quantum system described by the Hamiltonian $\hat{H}_0$ are constructed in [4]. To calculate the current (15), we shall use the following expressions from [4]:

$$\left.\begin{aligned} &\hat{H}_0 = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 \\ &\hat{H}_1 = \hbar\omega\left(\hat{A}_\alpha^+\hat{A}_\alpha^- + \frac{1}{2}\right); \quad \hat{H}_2 = \hbar\omega_0\left(\hat{A}_\beta^+\hat{A}_\beta^- + \frac{1}{2}\right), \quad \hat{H}_3 = \left(\frac{\omega_0}{\omega}\right)^2\frac{\hat{p}_y^2}{2m} \end{aligned}\right\} \quad (17)$$

$$\left.\begin{aligned} &\hat{A}_\alpha^\mp = \frac{1}{\sqrt{2\hbar}}e^{\pm i\omega t}\left[\sqrt{m\omega}(x - \hat{x}_0) \pm \frac{i\hat{p}_x}{\sqrt{m\omega}}\right], \quad \omega^2 = \omega_0^2 + \omega_c^2, \\ &\hat{A}_\beta^\mp = \frac{1}{\sqrt{2\hbar}}e^{\pm i\omega_0 t}\left[\sqrt{m\omega_0}z \pm \frac{i\hat{p}_z}{\sqrt{m\omega_0}}\right], \quad \hat{x}_0 = -\left(\frac{\omega_c}{\omega}\right)^2\frac{\hat{p}_y}{m\omega_c} \end{aligned}\right\} \quad (18)$$

$$\left[\hat{A}_i^-\hat{A}_k^+\right] = 1, \quad i = \alpha, \beta \quad (19)$$

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_0\right)\psi = 0, \quad \psi = |\alpha>|\beta>|k_y>, \quad |k_y> = e^{ik_y y} \quad (20)$$

$$\hat{A}_\alpha^-|\alpha> = \alpha|\alpha>, \quad \hat{A}_\beta^- = \beta|\beta>, \quad <\alpha|\alpha> = 1, \quad <\beta|\beta> = 1$$

α, β, k_y are the quantum numbers.

To calculate the current we adopt the scheme from [2]: express all quantities of the operators $\hat{A}^{\pm}_{\alpha}$, $A^{\pm}_{\beta}$; arrange the operators, replace the operators by their eigenvalues; integrate over α, β, k_y, using the standard integrals. We omit the terms proportional to the product $(\hat{A}^{+})^{p}(\hat{A}^{-})^{s}$ at $p\neq s$ and to k_y^{l} at l=1,3,5,…, as they give zero when integrated over α, β, and k_y respectively.

The first term in (15) equals to zero when integrated over k_y. Making the cyclic permutation we transform the second term in (15) to the form

$$Tr\,\hat{\rho}_0\left[\hat{V},y\right]=-\frac{\delta}{L_x}Tr\,\hat{\rho}_0\,x\left[\hat{H}_0,y\right] \tag{21}$$

Making use of equations (17) x can be expressed in terms $\hat{A}^{\pm}_{\alpha}$, $A^{\pm}_{\beta}$:

$$x=\hat{x}_A+\hat{x}_0,\quad \hat{x}_A=\sqrt{\frac{\hbar}{2m\omega}}\left(e^{i\omega t}\hat{A}^{+}_{\alpha}+e^{-i\omega t}\hat{A}^{-}_{\alpha}\right) \tag{22}$$

The integration over γ' in third term is reduced to

$$Tr\,\hat{\rho}_1\left[\hat{H}_0,y\right]=-Tr\hat{\rho}_0\left[\left(\frac{\delta\xi}{L_x}-\frac{\delta}{\gamma L_x}\right)x'-\frac{\delta}{2L_x}\left(\hat{H}_0x'+x'\hat{H}_0\right)-\frac{\delta}{2}\hat{H}_0\gamma\right] \tag{23}$$

The prime denotes that in $\hat{x}_A$ substitutions $\hat{A}^{-}_{\alpha}\rightarrow(C/\hbar\omega)\hat{A}^{-}_{\alpha}$, $\hat{A}^{+}_{\alpha}\rightarrow(C/\hbar\omega)\hat{A}^{+}_{\alpha}\,exp(\hbar\omega\gamma)$ and $x_0\rightarrow x_0\gamma$ must be done,

$$C=1-exp(-\hbar\omega\gamma) \tag{24}$$

Finally from equation (15) we derive

$$j_y=\frac{ien}{\hbar}\frac{\delta\gamma}{L_x}Tr\,\hat{\rho}_0(\hat{H}_0-\xi)\hat{x}_0\left[\hat{H}_0,y\right] \tag{25}$$

From (25) one can see that the zero-order term tends to zero. It is therefore enough to see the equilibrium grand partition function in equation (25).

It is easy to shown that

$$\left[\hat{H}_0,y\right]=-\frac{i\hbar}{m}\left(\frac{\omega_0}{\omega}\right)^2\hat{p}_y \tag{26}$$

Substituting (12), (17), (26), $\hat{x}_0$ from (18) into (25) and using the scheme for current calculation [2] we finally obtain

$$j_y=\left(\frac{\omega_c}{\omega}\right)^2\frac{nck}{H}\left(\frac{3}{2}-\xi\gamma+\frac{\hbar\omega\gamma}{2}coth\frac{\hbar\omega\gamma}{2}+\frac{\hbar\omega_0\gamma}{2}coth\frac{\hbar\omega_0\gamma}{2}\right)\frac{\delta T_0}{L_x} \tag{27}$$

As is seen from the comparison of equations (27) and (3) the coefficient at ($-\delta TL_x^{-1}$) coincides with the expression for β_{yx}.

Taking into account the expressions (43), (46) [2] we may write the entropy S of the parabolic QW directed perpendicular to the quantizing magnetic field. Introducing S in the expression for β_{yx} we derive the well known result for the β_{yx} in the nondegenerate case [5]:

$$\beta_{yx}=-\left(\frac{\omega_c}{\omega}\right)^2\frac{c}{H}S \tag{28}$$

It should be noted that as opposed to the previous researches (see, for example, [6]) given method of the effective Hamiltonian needs no account of the diamagnetism.

I wish to express my sincere thanks to Acad. Hashimzadeh F.M. for helpful discussion.

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TERMOMAQNİT CƏRƏYANLARI HESABLAMAQ ÜÇÜN YENİ METOD. KVANT MƏFTİLİ

Kvant məftilində qeyri-dissipativ termomaqnit cərəyanları hesablamaq üçün effektiv Hamiltonian metodu (EHM) təklif edilib. EHM-da mövcud ədəbiyyatdan fərqli olaraq temperatur Hamiltoniana daxil edilib. Hesablamalar koherent hallar təsvirində, parabolik kvant məftili və cırlaşmamış statistika üçün aparılmışdır.

Alınan termomaqnit tenzorunun qeyri-diaqonal tərkib hissəsi başqa üsullarla hesablanmış adı çəkilən tenzorun ifadəsi ilə üst-üstə düşür. Fərqli olaraq, EHM-dan istifadə etdikdə elektron diamaqnetizminin nəzərə alınmasına ehtiyac yaranmır.

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НОВЫЙ МЕТОД РАСЧЕТА ТЕРМОМАГНИТНОГО ТОКА. КВАНТОВАЯ ПРОВОЛОКА

Для расчета недиссипативного термомагнитного тока в квантовой проволоке предложен метод эффективного гамильтониана (МЭГ). В этом методе в отличие от предшествующих работ удается ввести температуру в гамильтониан. Расчеты произведены в представлении когерентных состояний для параболической квантовой проволоки и невырожденной статистики.

Полученное этим методом выражение для недиагональной компоненты термомагнитного тензора совпадает с известным из литературы выражением. Следует отметить, что при использовании МЭГ не возникает необходимости в учете диамагнетизма электронов.

Received: 17.09.09