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Flux rule, $U(1)$ instanton, and superconductivity

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Abstract We examine some consequences of the duality that a $U(1)$ phase factor added on a wave function describes a whole system motion and also plays the role of a $U(1)$ gauge potential. First, we show that the duality solves a long-standing puzzling problem that the ‘flux rule’ (the Faraday’s induction formula) and the Lorentz force calculation for an emf emerging in an electron system moving in a magnetic field give the same result (Feynman et al. [1]). Next, we examine a $U(1)$ phase factor induced on the wave function for an electron system due to the single-valuedness requirement of the wave function with respect to the electron coordinates, and its consequential appearance of a $U(1)$ instanton. This instanton explains the Meissner effect, supercurrent generation, flux quantization in the units of $\frac{h}{2e}$, and the voltage quantization in the units of $\frac{hf}{2e}$ across the Josephson junction in the presence of a radiation field with frequency f . In the experiment, a radiation field must be present to have a finite voltage across the Josephson junction; but a clear explanation for it has been lacking. The present work provides an explanation for it, and also explains the high precision of the quantized voltage as due to a topological effect.

Keywords Flux rule, $U(1)$ instanton

The role played by the electromagnetic gauge potential (vector+ scalar potentials) is different in quantum theory and classical theory. In classical theory, the gauge potential is a supplementary tool that can be used to facilitate calculations involving the magnetic field \mathbf{B}^{em} and electric field \mathbf{E}^{em} . On the other hand, it is a real physical entity in quantum theory. The physical reality of

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the gauge potential has been predicted [2] and experimentally verified [3]. The explanation of the Meissner effect observed in superconductors is explained using the London formula that directly connects the current density to the vector potential [4]. It is also notable that a new approach of electrodynamics using the quantum nature of matter with the gauge potential rather than using Maxwell's equations has been proposed [5].

From the view point that the vector potential \mathbf{A}^{em} and scalar one φ^{em} are more fundamental than \mathbf{B}^{em} and \mathbf{E}^{em} , two of Maxwell's equations, $\nabla \cdot \mathbf{B}^{\text{em}} = 0$ and $\nabla \times \mathbf{E}^{\text{em}} = -\frac{\partial \mathbf{B}^{\text{em}}}{\partial t}$ become the equations that define \mathbf{B}^{em} and \mathbf{E}^{em} from the fundamental gauge potential,

$$\mathbf{B}^{\text{em}} = \nabla \times \mathbf{A}^{\text{em}}; \quad \mathbf{E}^{\text{em}} = -\frac{\partial \mathbf{A}^{\text{em}}}{\partial t} - \nabla \varphi^{\text{em}} \quad (1)$$

The interaction of the quantum system and electromagnetic field is introduced by the following changes in the material Hamiltonian,

$$\mathbf{p} = \frac{\hbar}{i} \nabla \rightarrow \frac{\hbar}{i} \nabla - q \mathbf{A}^{\text{em}}; \quad i\hbar \frac{\partial}{\partial t} \rightarrow i\hbar \frac{\partial}{\partial t} - q\varphi^{\text{em}} \quad (2)$$

where $q = -e$ is the electron charge. This way of including the interaction gives rise to a duality that a $U(1)$ phase factor added on a wave function describes a whole system motion, and also works as a $U(1)$ gauge potential.

Let us see this point more, closely. We denote the wave function of a system with N_e electrons as $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_{N_e}, t)$, where \mathbf{x}_i is the coordinate of the i th electrons. We express it as a product form

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_{N_e}, t) = \Psi_0(\mathbf{x}_1, \dots, \mathbf{x}_{N_e}, t) \exp\left(-i \sum_{j=1}^{N_e} f(\mathbf{x}_j, t)\right) \quad (3)$$

where Ψ_0 is a wave function for a currentless state, and $\exp(-i \sum_{j=1}^{N_e} f(\mathbf{x}_j, t))$ describes the whole system motion. Ψ_0 may depend adiabatically on time through the adiabatic change of the frame, and the currentless here means with respect to this moving frame.

We can transfer the phase factor from the wave function to the Hamiltonian, resulting the modification of the gauge potential as $\mathbf{A}^{\text{em}} \rightarrow \mathbf{A}^{\text{em}} + \frac{\hbar}{q} \nabla f$ and $\varphi^{\text{em}} \rightarrow \varphi^{\text{em}} - \frac{\hbar}{q} \partial_t f$.

Then, we may regard

$$\mathbf{A}^{\text{eff}} = \mathbf{A}^{\text{em}} + \frac{\hbar}{q} \nabla f; \quad \varphi^{\text{eff}} = \varphi^{\text{em}} - \frac{\hbar}{q} \partial_t f \quad (4)$$

as the effective gauge potentials in the material. Actually, all the observables will be given as functionals of \mathbf{A}^{eff} and φ^{eff} instead of \mathbf{A}^{em} and φ^{em} since \mathbf{A}^{em} and φ^{em} always accompanied by ∇f and $\partial_t f$ in the above form.

In the present work, we identify \mathbf{A}^{eff} and φ^{eff} as the effective gauge potentials in the material; and also identify the observed magnetic and electric fields in it as

$$\mathbf{B}^{\text{eff}} = \nabla \times \mathbf{A}^{\text{eff}}; \quad \mathbf{E}^{\text{eff}} = -\frac{\partial \mathbf{A}^{\text{eff}}}{\partial t} - \nabla \varphi^{\text{eff}} \quad (5)$$

Using the above identifications, we first explain a puzzling fact that the ‘flux rule’ (the Faraday’s induction formula) can be used for the calculation of the electromotive force (emf) emerging in an electron system moving in a magnetic field and gives the same result calculated by the Lorentz force [1]. Next we take up superconductivity. It has been shown that when spin-vortices are created by itinerant electrons, the currentless wave function Ψ_0 becomes multi-valued with respect to the electron coordinates [6, 7]; and a phase factor is induced to make Ψ single-valued. This induced phase factor creates a $U(1)$ instanton in the material, and gives rise to phenomena associated with superconductivity.

Firstly, we derive some general relations obtained using \mathbf{A}^{eff} and φ^{eff} for later use (some of them are also found in Ref. [8]). Using the fact that \mathbf{A}^{em} and φ^{em} appear as part of \mathbf{A}^{eff} and φ^{eff} , the current density \mathbf{j} and charge density ρ are given by

$$\mathbf{j} = -\frac{\delta E}{\delta \mathbf{A}^{\text{em}}} = -\frac{q}{\hbar} \frac{\delta E}{\delta \nabla f}; \quad \rho = \frac{\delta E}{\delta \varphi^{\text{em}}} = \frac{q}{\hbar} \frac{\delta E}{\delta \partial_t f}, \quad (6)$$

From Eq. (6), the canonical conjugate variable for f is given by

$$p_f = \hbar q^{-1} \rho, \quad (7)$$

Then, using p_f , the Lagrangian for f is given by

$$L = - \int d^3x \rho \varphi^{\text{eff}} - \bar{E} [\mathbf{A}^{\text{eff}}] \quad (8)$$

where \bar{E} is defined as a functional of only \mathbf{A}^{eff} as

$$\bar{E} [\mathbf{A}^{\text{eff}}] = E [\mathbf{A}^{\text{eff}}, \varphi^{\text{em}}] - \int d^3x \rho \varphi^{\text{em}} \quad (9)$$

The Hamilton’s equations for f and p_f are given by

$$\dot{p}_f = -\frac{\delta E}{\delta f} = \nabla \cdot \frac{\delta E}{\delta \nabla f} \quad (10)$$

$$\dot{f} = \frac{\delta E}{\delta p_f} = \frac{q}{\hbar} \frac{\delta E}{\delta \rho} \quad (11)$$

where the fact that E depends not directly on f but through ∇f and $\partial_t f$ is used.

Using Eqs. (6) and (7), Eq. (10) becomes the equation for the conservation of charge $\dot{\rho} = -\nabla \cdot \mathbf{j}$.

For the ground state of an isolated system, Eq. (11) gives $\hbar \dot{f} = 0$ since the energy is optimized with respect to ρ . If the system is contacted with a particle

reservoir, it indicates that $\hbar\dot{f}$ is the chemical potential. In this case, $\hbar\dot{f}$ is fixed by the constraint $\int d^3x\rho = qN_e$, where N_e is the number of electrons in the system.

Now, let us examine the validity of using the ‘flux rule’ (the Faraday’s induction formula) for the calculation of an emf emerging in an electron system moving in a magnetic field [1]. We consider a moving crossbar on a U-shaped rail by changing the area surrounded by the circuit composed of the U-shaped rail and the crossbar [1]. An emf is induced in this circuit when it is penetrated by a magnetic field. A puzzling fact is that this emf can be calculated classically either by the Lorentz force acting on electrons in the crossbar or by the Faraday’s induction formula as the time-derivative of the flux through the circuit. This is puzzling since the two methods used here are different in the physical origin in the classical theory [1].

Let us place the circuit of the moving bar and the U-shaped rail in the xy plane and the magnetic field is applied in the z direction. Then, the magnetic field is by $(0, 0, B)$. The crossbar is parallel to the x axis and moving in the y direction with velocity v . The wave function for an electron in the crossbar is expressed as $\Psi_0(x, y - y_0(t), z)$ when $B = 0$, where $y_0(t) = vt$ is the center of the y -coordinate of the moving bar ($y_0 = 0$ is the position of the crossbar at $t = 0$) by assuming that the wave function adiabatically depends on $y_0(t)$ [9].

We express the wave function for the case when $B \neq 0$ as $\Psi(x, y, z, t) = \Psi_0(x, y - y_0(t), z)e^{-if(x, y, z, t)}$. We choose the gauge in which the vector potential for the applied magnetic field is given by $\mathbf{A}^{\text{em}} = (0, Bx, 0)$. We obtain f by minimizing the energy calculated by Ψ , $\langle \Psi_0 | H[\mathbf{A}^{\text{eff}}] | \Psi_0 \rangle$ (H is the Hamiltonian depends on $\mathbf{A}^{\text{eff}} = \mathbf{A}^{\text{em}} - \hbar e^{-1} \nabla f$). From the stationary condition of the energy with respect to the variation in ∇f , we will obtain $\mathbf{A}^{\text{eff}} = 0$ since $\mathbf{A}^{\text{em}} \neq 0$ increases the kinetic energy. This leads to the solution $\nabla f = (0, \hbar^{-1}eBx, 0)$. Then, the wave function $\Psi(x, y, z, t)$ is given by

$$\Psi(x, y, z, t) = \Psi_0(x, y - y_0(t), z) \exp\left(-i\frac{eB}{\hbar}xy\right) \quad (12)$$

Actually, this wave function agrees with the one obtained by using the Dirac’s magnetic phase factor [10,11] (the same phase factor can be found as in Eq. (15.29) of Ref. [1]).

Due to the fact that f is obtained by the stationary condition of $\langle \Psi_0 | H[\mathbf{A}^{\text{eff}}] | \Psi_0 \rangle$ with respect to the variation of ∇f , we have

$$j_y = -\frac{\delta \langle \Psi | H[\mathbf{A}^{\text{em}}] | \Psi \rangle}{\delta A_y^{\text{em}}} = -\frac{\delta \langle \Psi_0 | H[\mathbf{A}^{\text{eff}}] | \Psi_0 \rangle}{\delta A_y^{\text{em}}} = -\frac{e}{\hbar} \frac{\delta \langle \Psi_0 | H[\mathbf{A}^{\text{eff}}] | \Psi_0 \rangle}{\delta (\partial_y f)} = \text{⑩} \quad (13)$$

where j_y is the current density in the y direction. Therefore, our choice of $\mathbf{A}^{\text{em}} = (0, Bx, 0)$ correctly describes the situation where the electric current of the electromagnetic field origin in the y direction is absent.

Now we assume that the width of the moving bar in the y direction is very small. Then, we may use the approximation, $y \approx y_0 = vt$. Consequently,

$\Psi(x, y, z, t)$ is expressed as

$$\Psi(x, y, z, t) \approx \Psi_0(x, y - y_0(t), z) \exp\left(-i \frac{eB}{\hbar} xvt\right). \quad (14)$$

From the phase factor of the wave function in Eq. (14), the time-derivative of the x component of the momentum $p_x = \hbar k_x$ is given by

$$\dot{p}_x = \hbar \dot{k}_x = -eB\dot{y}_0 = -eBv \quad (15)$$

This shows that the force $-eBv$ is acting on the electron in the x direction. This force equals the Lorentz force (*the Lorentz force result*).

The same problem is also solved by transferring the phase factor $\exp(-i \frac{eB}{\hbar} x y_0(t))$ into the Hamiltonian. It gives rise to the x component of an effective vector potential $A_x^{\text{eff}} = -Bvt$. The electric field is then calculated using Eq. (5) as

$$E_x^{\text{eff}} = -\partial_t A_x^{\text{eff}} = Bv, \quad (16)$$

This is the electric field of the emf calculated by the flux rule (*the flux rule result*). The force acting on the electron by the emf is calculated as $F_x = -eBv$, which is equal to the value in Eq. (15). The reason that the two different methods of calculations give the same result is attributed to the dual role played by the $U(1)$ phase on the wave function.

Next, we consider the emergence of a $U(1)$ instanton in materials, and the appearance of various phenomena associated with superconductivity. It has been shown that when itinerant electrons form spin-vortices, the currentless wave function Ψ_0 in Eq. (3) obtained by energy minimization becomes multi-valued with respect to the electron coordinates [6,7]. In this situation, the single-valued requirement of the total wave function Ψ induces a phase factor that describes the whole system motion with $f = \frac{1}{2}\chi$ in Eq. (3), where χ is an angular variable with period 2π [6,7].

The equation to determine χ is given as the stationary condition for the following functional

$$F[\nabla\chi] = E[\mathbf{A}^{\text{eff}}, \varphi^{\text{em}}] + \sum_{\ell=1}^{N_{\text{loop}}} \lambda_{\ell} \left(\oint_{C_{\ell}} \nabla\chi \cdot d\mathbf{r} - 2\pi\bar{w}_{\ell} \right) \quad (17)$$

with respect to the variation of $\nabla\chi$, where the second term in the rhs of Eq. (17) imposes the constraint for the single-valuedness of the total wave function, and λ_{ℓ} 's are Lagrange multipliers [6,7].

The stationary condition yields,

$$0 = \frac{\delta E[\mathbf{A}^{\text{eff}}, \varphi^{\text{em}}]}{\delta \nabla\chi} + \sum_{\ell=1}^{N_{\text{loop}}} \lambda_{\ell} \frac{\delta}{\delta \nabla\chi} \oint_{C_{\ell}} \nabla\chi \cdot d\mathbf{r}. \quad (18)$$

The solution $\nabla\chi$ is a $U(1)$ 'instanton',

$$\mathbf{A}^{\text{fic}} = \frac{\hbar}{2q} \nabla\chi \quad (19)$$

in the sense that it is a solution of a classical equation of motion (i.e., Eq. (18)) and characterized by topological quantum numbers \bar{w}_ℓ given by $\bar{w}_\ell = w_\ell[\chi] \equiv (2\pi)^{-1} \oint_{C_\ell} \nabla\chi \cdot d\mathbf{r}$ as is given in the constraint in Eq. (17) [12].

If the instanton with $w_\ell[\chi] \neq 0$ emerges, we have $\lambda_\ell \neq 0$. Then, using Eq. (6) with $f = \frac{1}{2}\chi$ and Eq. (18)), a nonzero current density

$$\mathbf{j} = \frac{2q}{\hbar} \sum_\ell \lambda_\ell \frac{\delta}{\delta \nabla\chi} \oint_{C_\ell} \nabla\chi \cdot d\mathbf{r} \quad (20)$$

is obtained. This is a persistent current that flows as long as the instanton exists. The current carrying state with the instanton is higher in energy than the currentless state; however, the single-valued requirement of the wave function insists the presence of the instanton, the current carrying state is the only allowed state.

The functional in Eq. (17) can be extended to the case where a current is fed, externally [6, 7]. In such a case, the external current can flow through the system without a voltage drop, thus, it is a supercurrent.

The Meissner effect is explained as follows. If $\nabla\chi$ is optimized neglecting the constraint, a currentless state (i.e., a state with $\mathbf{j} = 0$) is obtained in the same reason we obtained Eq. (13). The energy $E[\mathbf{A}^{\text{eff}}, \varphi^{\text{em}}]$ for this state should be no more than the energy for the state with $\mathbf{j} \neq 0$ obtained including the constraint. Further, \mathbf{A}^{eff} is gauge invariant with respect to the choice of the gauge for \mathbf{A}^{em} since $\nabla\chi$ is obtained through optimization and this optimization compensates the arbitrariness of the gauge in \mathbf{A}^{em} [6, 7]. Thus, for small \mathbf{A}^{eff} , the energy functional is given as a quadratic functional of the gauge invariant \mathbf{A}^{eff} ; then, the current density is a linear functional of \mathbf{A}^{eff} [8]. Therefore, the state with $\mathbf{A}^{\text{eff}} = 0$ is currentless. The linear relation between the current and \mathbf{A}^{eff} leads to the Meissner effect.

As is well-known, the Meissner effect gives rise to the flux quantization. Let us re-derive this: we take a ring-shaped system and consider a loop C that encircles the hole of the ring through the bulk of the ring. We assume $\mathbf{A}^{\text{eff}} = 0$ along C due to the Meissner effect. Then, we have

$$\oint_C \mathbf{A}^{\text{em}} \cdot d\mathbf{r} = -\frac{\hbar}{2(-e)} \oint_C \nabla\chi \cdot d\mathbf{r} = \frac{\hbar}{2e} n \quad (21)$$

where n is an integer corresponding to the topological winding number of χ around C . This shows the flux quantization in the units of $\frac{\hbar}{2e}$. The quantization arises from the topological property of $\mathbf{A}^{\text{fic}} = \frac{\hbar}{2q} \nabla\chi$.

Lastly, we consider the ac Josephson effect [13]. The most clear experimental observation of the ac Josephson effect is the appearance of plateaus in the I - V plot under the application of a microwave radiation with dc current feeding [14]. The voltage V at the plateaus is given by $V = \frac{\hbar f}{2e} n$ (n is an integer), where f is the applied microwave frequency.

We now explain the observed voltage quantization using the $U(1)$ instanton in the xt plane. Let us consider a Josephson junction (or an SIS junction) which is composed of two superconductors ‘ S_L ’ and ‘ S_R ’, and a non-superconducting

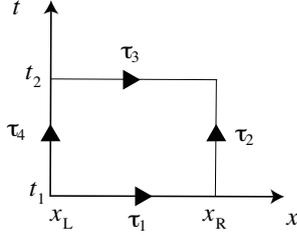


Fig. 1 Loop for the voltage quantization calculation. The SIS junction is along the x direction; the edges of the left ‘S’ (‘ S_L ’) and right ‘S’ (‘ S_R ’) that contact with ‘I’ are denoted as x_L and x_R , respectively. t_2 and t_1 are two times with separation $t_2 - t_1 = 1/f$, where f is the frequency of the radiation field applied.

region ‘I’ between them. We take the direction of the junction in the x direction and the edges of ‘ S_L ’ and ‘ S_R ’ contacting with ‘I’ as x_L and x_R , respectively (Fig. 1). We apply a microwave with an electric field $E_x^{\text{em}} = E_0 \cos(2\pi ft)$ where E_0 is a constant.

Then, the effective electric field in ‘I’ is given by

$$E_x^{\text{eff}} = -\frac{\partial A_x^{\text{eff}}}{\partial t} - \partial_x \varphi^{\text{eff}} = E_x^{\text{em}} - \frac{\hbar}{2q} (\partial_t \partial_x - \partial_x \partial_t) \chi \quad (22)$$

The voltage across the junction V is calculated as an average voltage calculated using E_x^{eff} over the time interval $1/f$,

$$V = f \int_{t_1}^{t_2} dt \int_{x_L}^{x_R} dx E_x^{\text{eff}} = f \int_{t_1}^{t_2} dt \int_L^R dx E_x^{\text{em}} - \frac{\hbar f}{2q} \int_{t_1}^{t_2} dt \int_{x_L}^{x_R} dx (\partial_t \partial_x - \partial_x \partial_t) \chi \quad (23)$$

where t_2 and t_1 are two times with separation $t_2 - t_1 = 1/f$, and f is the frequency of the radiation field.

We have $\int_{t_1}^{t_2} dt E_x^{\text{em}} = 0$, and the presence of the instanton in the xt plane yields,

$$\int_{t_1}^{t_2} dt \int_{x_L}^{x_R} dx (\partial_t \partial_x - \partial_x \partial_t) \chi = 2\pi n \quad (24)$$

where n is an integer.

Thus, V is given by

$$V = -f \frac{\hbar}{2(-e)} 2\pi n = \frac{\hbar f}{2e} n \quad (25)$$

As indicated in Eq. (24), this quantized voltage is a topological origin in a similar manner as the quantized Hall conductance in the quantum Hall effect [15] and the flux quantization in Eq. (21).

Let us examine how this instanton looks like. We consider the loop in the xt plane shown in Fig. 1, where $\tau_1 = \chi(x_R, t_1) - \chi(x_L, t_1)$, $\tau_2 = \chi(x_R, t_2) - \chi(x_R, t_1)$, $\tau_3 = \chi(x_R, t_2) - \chi(x_L, t_2)$, and $\tau_4 = \chi(x_L, t_2) - \chi(x_L, t_1)$. Then, the condition in Eq. (24) is given by $\tau_1 + \tau_2 - \tau_3 - \tau_4 = 2\pi n$.

The classical action S from which the instanton solution is obtained is given by $S(\tau_1, \tau_2, \tau_3, \tau_4) = \int_{t_1}^{t_2} L dt$. The optimization of S is done under the constraint $\tau_1 + \tau_2 - \tau_3 - \tau_4 = 2\pi n$. This is achieved by using the following function

$$P(\tau_1, \tau_2, \tau_3, \tau_4, \lambda) = S - \lambda(\tau_1 + \tau_2 - \tau_3 - \tau_4 - 2\pi n) \quad (26)$$

where λ is a Lagrange multiplier.

From the stationary condition of P with respect to variations of $\tau_i, i = 1, 2, 3, 4$, and using the relations in Eq. (6), we have

$$\begin{aligned} \lambda &= \frac{\partial S}{\partial \tau_1} = \frac{\partial S}{\partial \tau_2} = -\frac{\partial S}{\partial \tau_3} = -\frac{\partial S}{\partial \tau_4} \\ &= \frac{\hbar}{2e} J(t_1) = -\frac{\hbar}{2e} Q_R = -\frac{\hbar}{2e} J(t_2) = \frac{\hbar}{2e} Q_L, \end{aligned} \quad (27)$$

where $J(t_1)$ and $J(t_2)$ are the current flowing from x_L to x_R at time t_1 and t_2 , respectively; and Q_R and Q_L are charges at x_R and x_L , respectively. The above relation shows that $Q_R = -Q_L$, thus, the instant has charges of the same magnitude and opposite sign at its end points. This is similar to a flux tube having magnetic monopoles of the same magnitude and opposite sign at its end points [16].

Now consider the role played by the dc current feeding in the voltage quantization. Since the instantons in the xt plane have charges of the same magnitude and opposite sign at the two ends, the junction behaves a capacitor. We denote the capacitance of it as C and the stored charge as Q , with the relation $Q = CV_n$, where V_n is the voltage given in Eq. (25).

The junction is not a perfect capacitor; the tunneling causes the discharging by the recombination of the opposite charges. We may express this process by $\frac{dQ}{dt} = -\alpha Q$, where α is the discharging rate. By including the current flow due to the tunneling \bar{J} and the feeding current from the lead J , the conservation of the charge gives the following relation,

$$\frac{dQ}{dt} = J - \bar{J} - \alpha Q. \quad (28)$$

The stationary condition $\frac{dQ}{dt} = 0$ yields $J = \alpha CV_n + \bar{J}$; thus, the observed $I - V$ plateaus in the experiment is obtained [14]. Here, the dc current feeding helps to create instantons that are destroyed due to the pair-annihilation of the charges by supplying charges.

In the Josephson's prediction [13], an application of a dc voltage V on the junction is assumed. However, a simple application of a dc voltage results in the flow of a dc current with zero voltage across the junction. Experiments indicate that a radiation field is necessary to have a voltage across the junction

[14]. The present theory explains that a radiation field is necessary to create the $U(1)$ instanton.

In conclusion, we show that the duality of a $U(1)$ phase factor added on a wave function, a whole system motion and a $U(1)$ gauge potential, explains the validity of using the ‘flux rule’ (the Faraday’s induction formula) for the calculation of an emf emerging in an electron system moving in a magnetic field. This duality allows the appearance of a $U(1)$ instanton in materials, and explains the phenomena associated with superconductivity as topological phenomena brought about by the instanton.

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