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**HOPPING RATE OF LOCALIZED DEFECTS INTERACTING WITH
TWO-DIMENSIONAL ELECTRON SYSTEMS IN A MAGNETIC
FIELD**

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Abstract

The hopping rate of localized defects interacting with a two-dimensional electron system is studied. It is shown that, at low temperatures, the hopping rate is an oscillatory function of the inverse of the magnetic field. The period and the amplification of the oscillations are independent of the electron-defect interaction and the detailed structure of the sample. It is predicted that the temperature dependence of the hopping rate differs significantly between the cases of filled and half filled Landau levels.

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Localized defects in solids (e.g., muons in metals or muoniums in semiconductors) presents an interesting problem in condensed matter physics.¹⁻⁵ Due to the nonvanishing offdiagonal matrix elements of the Hamiltonian, these defects can hop from one potential well to a neighboring one. When they hop, the environment can be excited (e.g., electronic excitations and phonons). Even a slowly moving heavy charged particle in a degenerate Fermi gas can excite electron-hole pairs with small excitation energy. These low energy electrons are not able to rearrange themselves so that their wavefunction are centered around the new site. As a result, the hopping bandwidth is greatly reduced. This result is a consequence of the "Anderson orthogonality catastrophe".⁶ This comes about as a result of the presence of a large number of electron-hole pairs of low excitation energy that must be accounted for within the structure of the many-particle wavefunction in the basis of electronic eigenstates. By assuming a model electron-particle interaction V_0 , and a constant density of states ρ of width D for conduction electrons, Kondo found that the hopping rate is proportional to T^{2K-1} , where $K = V_0^2 \rho^2 (1 - \sin^2 k_F a / (k_F a)^2)$. Here a is the nearest neighbor hopping distance and k_F is the Fermi wavevector. This can be understood as follows: T^{2K} comes from the effect of the screening of electrons whereas T^{-1} comes from the level broadening proportional to T . Experimentally, this T^{2K-1} behavior was observed by Kadono *et al* in muon diffusion in Cu.^{7,8}

By treating the dynamically screened fields of electrons selfconsistently, we have shown in a recent work⁹ that the reduction of the hopping bandwidth is not only due to the wavefunction overlap but comes from all possible electronic virtual excitations. The plasmon excitation contributes a normalization factor which can be as large as one to two orders of magnitude in normal metals.

In this letter, we shall study the hopping of localized defects in a structure where electrons are confined in a two-dimensional (2D) or quasi 2D plane and are under a constant magnetic field perpendicular to the plane. We shall show that the hopping rate can exhibit some new features quite distinct from the case where electrons are free particles. Due to the unique properties of 2D systems under a magnetic field, our study provides a method of modulating the motion of the defects by varying the applied field. On the other hand, it is also suggested that one may study the properties of the electrons (e.g., density of states) via the motion of the defects. The structure used here can be a heterostructure, a double barrier structure with a thin well in between. Electrons are assumed to be confined in the direction perpendicular to the plane.

The transition probability of a particle in eigenstate $|i\rangle$ hopping from lattice site 1 to lattice site 2 in eigenstate $|f\rangle$ is given by ^{2,10}

$$\nu = 2J_0^2 \int_0^\infty dt \langle e^{\frac{i}{\hbar} H_i t} e^{-\frac{i}{\hbar} H_f t} \rangle \quad (1)$$

where J_0 is the hopping band width. The average appearing in Eq. (1) is carried out over all possible initial states. In writing Eq. (1), it is assumed that the energy levels for a particle at lattice sites 1 and 2 are virtually the same, or the energy difference between corresponding energy levels at the two lattice sites is small compared to the temperature.

The initial Hamiltonian H_i is given by (assuming spin degeneracy)

$$H_i = H_c + V_1 \quad (2)$$

where

$$H_e = \sum_{n, k_y} \left(n + \frac{1}{2} \right) \hbar \omega_c a_{n, k_y}^\dagger a_{n, k_y} + U +$$

$$\frac{1}{2} \sum_{\vec{q}, k_y, k_y'} \sum_{nm, n'm'} v_q J_{nm}(q_x, k_y + q_y, k_y) J_{n'm'}(-q_x, k_y' - q_y, k_y') a_{n, k_y + q_y}^\dagger a_{n', k_y' - q_y}^\dagger a_{m', k_y'} a_{n', k_y}. \quad (3)$$

Here U is a potential due to short-range scatterers and V_1 is the electron-defect interaction when the defect is at position (z_1, \vec{R}_1) given by,

$$V_1 = \sum_{\vec{q}} V_q e^{-q z_1} e^{i\vec{q} \cdot \vec{R}_1} J_{nn'}(q_x, k_y, k_y - q_y) a_{n, k_y}^\dagger a_{n', k_y + q_y} \quad (4)$$

In these equations the symbol J_{nm} is given by

$$J_{nm}(q_x, k_y, k_y') = \int_{-\infty}^{\infty} dx e^{iq_x x} \varphi_n \left(\frac{x}{l} + lk_y \right) \varphi_m \left(\frac{x}{l} + lk_y' \right) \quad (5)$$

where the following notations have been used, $\omega_c = eB/m$ is the cyclotron frequency, $l^2 = 1/(m\omega_c)$ is the magnetic length and $x_o = l^2 k_y$ is the center coordinate. The coordinate \vec{R} is along the x-y plane and z is along the third direction perpendicular to the plane. The function $\varphi_n(x)$ is the n th eigenfunction of a simple harmonic oscillator, a_{n, k_y}^\dagger and a_{n, k_y} are creation and destruction operators for an electron with quantum number n and k_y and $v_q = 4\pi e^2/q^2$ is the Fourier transform of the Coulomb interaction. In the following, we take $\vec{R}_1 = 0$ and $\vec{R}_2 = \vec{R}$. In the interaction representation

$$\phi(t) \equiv \langle e^{iH_e t} e^{-iH_e t} \rangle = \langle \hat{T} \exp[i \int_0^t d\tau V(\tau)] \rangle \quad (6)$$

where \hat{T} is the time-ordering operator, $V(t) \equiv e^{iH_e t} V e^{-iH_e t}$ and V is defined as

$$V = V_2 - V_1 = \sum_{\vec{q}} u_q J_{nn'}(q_x, k_y, k_y - q_y) a_{n, k_y}^\dagger a_{n', k_y + q_y} \quad (7)$$

with $u_q = V_q [e^{-q z_2} e^{i\vec{q} \cdot \vec{R}} - e^{-q z_1}]$. Expanding $\phi(t)$, keeping only the lowest order term, we obtain

$$\phi(t) = \exp[F(t)], \quad (8)$$

where

$$F(t) = - \int_{t > t_1 > t_2} dt_1 dt_2 \langle V(t_1) V(t_2) \rangle = - \int_{t > t_1 > t_2} dt_1 dt_2 \sum_{\vec{q}, \vec{q}'} V_q V_{q'}^* \langle n(\vec{q}, t) n(\vec{q}' t') \rangle. \quad (9)$$

Here $n(\vec{q}, t) = \sum J_{nn'}(-q_x, k_y, k_y + q_y) a_{n, k_y}^\dagger(t) a_{n', k_y + q_y}(t)$ is the density operator. In our calculations, we keep terms up to order u_q^2 . Therefore, the average in $F(t)$ can be replaced by the average over H_e . The density-density response function, by its definition, is given by

$$\langle n(\vec{q}, t) n(\vec{q}' t') \rangle = \delta(\vec{q} - \vec{q}') \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega(t-t')}}{1 - e^{-\beta\omega}} \Im \left[\frac{1}{\epsilon(\vec{q}, \omega)} \right] \quad (10)$$

where $\beta = T^{-1}$. In the random-phase-approximation (RPA),

$$\varepsilon(q, \omega) = 1 - v_q \chi(q, \omega) \quad (11)$$

and the single-particle density-density response function is

$$\chi_q(\omega) = \sum_{n, n'} C_{nn'}(q) \Pi_{nn'}(\omega) \quad (12)$$

where for ($n' > n$),

$$C_{nn'}(q) = \sum_{k_y} J_{nn'}(q_x, k_y, k_y - q_y) J_{n'n}(-q_x, k_y - q_y, k_y) = p \frac{n!}{n'!} X^{n'-n} e^{-X} [L_n^{n'-n}(X)]^2 \quad (13)$$

with $p = (2eB)/(\pi\hbar c)$, $X = (ql)^2/2$, and $L_n^m(X)$ is the associated Laguerre polynomial. The function Π is defined as

$$\Pi_{nn'}(\omega) = \frac{1}{\beta} \sum_l G_n(\omega_l + \omega) G_{n'}(\omega_l) \quad (14)$$

where $\omega_l = i(2l+1)T$. The single particle Green's function is given as $G_n(\omega) = [\hbar\omega - (n+1/2)\hbar\omega_c - \Sigma]^{-1}$. It should be noted that all quantities used here are retarded ones. We shall assume that the electronic selfenergy is due to some short-range scatterers and we will treat it within self-consistent Born approximation (SCBA). It can be shown^{11,12,13} that both G and Σ are diagonal in the Landau representation and they are independent of x_o . Furthermore, for short-range scattering, Σ is independent of n , i.e., a multiple of unit operator and it is determined by $\Sigma = \Gamma^2 \sum G_n(\omega)$, where $\Gamma^2 = (2/\pi)(\hbar^2\omega_c/\tau)$ and τ is the lifetime for zero magnetic field. By a standard technique¹², one can obtain

$$\Sigma(\omega) = \sum_n \frac{\Gamma^2}{\hbar\omega - (n+1/2)\hbar\omega_c - \Sigma(\omega)} \quad (15)$$

Single-Particle Excitations — Inserting this result in $F(t)$ and integrating over t_2 and t_1 , the term linear in t has no contribution. We obtain

$$F_{sp}(t) \approx 2 \sum_{\vec{q}} |u_{\vec{q}}|^2 \int \frac{d\omega}{\omega^2} \frac{1 - e^{-i\omega t}}{1 - e^{-\beta\omega}} \frac{\Im\chi(q, \omega)}{|\varepsilon_{\vec{q}}(\omega)|^2} \quad (16)$$

where \Im stands for the imaginary parts. It can be seen that the ω -integration is dominated by a region around $\omega \sim 0$. At small ω , $\Im[\chi] \propto \omega$ and static screening is applicable. In this case, the integration over ω can be carried out and we obtain

$$F_{sp}(t) = \int_0^\infty \frac{d^2q}{(2\pi)^2} \frac{|u_{\vec{q}}|^2}{|\varepsilon_{\vec{q}}|^2} \left[\frac{\Im\chi(q, \omega)}{\omega} \right]_{\omega < \xi} \left[\ln \left\{ \frac{\sinh \pi T t}{\pi T t} \sqrt{1 + \xi^2 t^2} \right\} + i \tan^{-1} \xi t \right], \quad (17)$$

where ξ is the cutoff which determines the range over which $\Im\chi_q(\omega) \sim \omega$ is valid. For large t , we obtain

$$\phi_{sp}(t) \approx (T/\xi)^{2K} \exp(-2\pi K T |t|) \exp(-i\pi K \text{sgn}(t)). \quad (18)$$

*The parameter K is defined as

$$K \equiv \int_0^\infty \frac{d^2 q}{(2\pi)^2} \left| \frac{u_q}{\epsilon_q} \right|^2 \left[\frac{\Im \chi(q, \omega)}{\omega} \right]_{\omega < \xi} \quad (19)$$

Upon using $\Im \Pi_{nn'}(\omega) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon [f(\epsilon) - f(\epsilon + \omega)] \Im [G_n(\epsilon + \hbar\omega)] \Im [G_n'(\epsilon)]$ we obtain

$$\left[\frac{\Im \chi(q, \omega)}{\omega} \right]_{\omega < \xi} = \int d\epsilon \frac{\partial f}{\partial \epsilon} \sum_{n, n'} C_{nn'}(q) \Im [G_n(\epsilon)] \Im [G_n'(\epsilon)] \quad (20)$$

where $f(\epsilon) = [\exp((\epsilon - \mu)/T) + 1]^{-1}$ is the Fermi distribution function and μ is the chemical potential to be determined selfconsistently through $N = (m\tau/\pi\hbar^3) \int d\epsilon f(\epsilon)\gamma(\epsilon)$. By converting the sum into a countour integral, we obtain ($\Sigma = \Delta + i\gamma$),

$$\left[\frac{\Im \chi(q, \omega)}{\omega} \right]_{\omega < \xi} = \int d\epsilon \frac{\partial f}{\partial \epsilon} C_{\bar{n}\bar{n}}(q) \frac{\pi^2}{(\hbar\omega_c)^2} \left[\frac{\sinh(2\pi\gamma/\hbar\omega_c)}{\cosh(2\pi\gamma/\hbar\omega_c) - \cos(2\pi(\epsilon - \Delta)/\hbar\omega_c - \pi)} \right]^2$$

where $\bar{n} = \epsilon/\omega_c$ and use has been made of the approximation $\mu \gg \Delta, \gamma$. This quantity is an oscillatory function of the inverse magnetic field. The amplitudes of oscillations increase with increasing magnetic field and decreasing temperature, but independent of detailed electron-defect interaction. In the low field limit, $\gamma/\hbar\omega_c > 1$, the quantity inside the square bracket becomes nearly sinusoidal

$$1 + \exp \left[-\frac{2\pi}{\omega_c \tau} \right] \cos \left(\frac{2\pi\epsilon}{\hbar\omega_c} - \pi \right).$$

In Eq.(19), $\epsilon_q = 1 + q_s/q$ is the static dielectric function, where the screening wavenumber $q_s = 2\pi e^2(\partial N/\partial \mu) = (2\pi e^2 m\tau/\pi\hbar^3) \int d\epsilon (\partial f/\partial \epsilon)\gamma$ which is also an oscillatory function of $1/B$.

Plasmon Excitation — We now turn to the contribution to $F(t)$ due to magnetoplasmon excitations. In the long wavelength limit, our calculations show that

$$F_{pl}(t) = 2 \sum_{\vec{q}} \frac{|u_q|^2}{v_q} \frac{\pi(1 - e^{-i\omega_p(q)t})}{\omega_p(q)^2(1 - e^{-\beta\omega_p(q)})} \left(\frac{\partial \Re \epsilon_q(\omega)}{\partial \omega} \right)_{\omega=\omega_p(q)}^{-1} \quad (21)$$

where \Re stands for the real parts and $\omega_p(q) = [(2\pi N e^2 q/m) + \omega_c^2]^{1/2}$ is the plasmon frequency. The oscillatory term $e^{-i\omega_p t}$ has no contribution to the t -integration. Therefore, F_{pl} is independent of time. Furthermore, the term $e^{-\beta\omega_p(q)}$ can be neglected at low temperature (note $\omega_p(q)$ is finite even at $q = 0$ due to applied magnetic field).

Therefore, $F_{pl} \approx \pi \sum_{\vec{q}} \frac{u_q^2}{v_q \omega_p(q)}$ only depends on the electron-defect interaction and decreases with the magnetic field. Our final result for the hopping rate can be written as

$$\nu = (J_0^2/\xi) e^{-F_{pl}} \frac{\cos \pi K}{\pi K} (T/\xi)^{2K-1}. \quad (22)$$

This result, although having the same functional form as in the bulk case, contains several new features. (i) For a defect trapped at distance z from the electron

plane, the electron-defect interaction is greatly reduced by a factor $\exp(-k_F z)$. As a result, $K \ll 1$ and the effect due to wavefunction overlap disappears. We have $\nu = J_0^2 \exp(-F_{pl}) / (TK)$, which is independent of the choice of ξ . (ii) ν is an oscillatory function of $1/B$, its mean value increases slowly with magnetic field due to magnetoplasmon excitation. A model calculation is performed by assuming only one electron layer and a positively charged defect at $z = 50A$ from the electron layer. Generalization to many-layer structure is quite straightforward. (iii) The temperature-dependence of the hopping rate now depends on the filling of the Landau levels. Because the amplitudes of oscillation in K increase with decreasing temperature, for integer fillings (minima in K) the rate increases faster than T^{-1} with decreasing temperature while for half integer fillings (maxima in K) the rate increases slower than T^{-1} . These two cases are shown in Fig.2.

In conclusion, we have proposed an investigation to study the hopping of localized defects in low dimensional systems. New features concerning the field-dependence and temperature-dependence of the hopping rate are predicted.

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Figure Captions

Fig.1. Plot of hopping rate as a function of magnetic field. The rate is normalized by its zero field value, $T=5K$, $\hbar\tau^{-1} = 0.015meV$, $R = 3A$ $z_1 = 50A$ and $z_2 = 52A$. The zero field Fermi energy is chosen to be $E_F = 12meV$.

Fig.2. Plot of hopping rate as a function of temperature for $E_F/\hbar\omega_c = 10$ (upper curve) and $E_F/\hbar\omega_c = 10.5$ (lower curve). The parameters E_F , τ , R , z_1 and z_2 are same as in Fig.1.

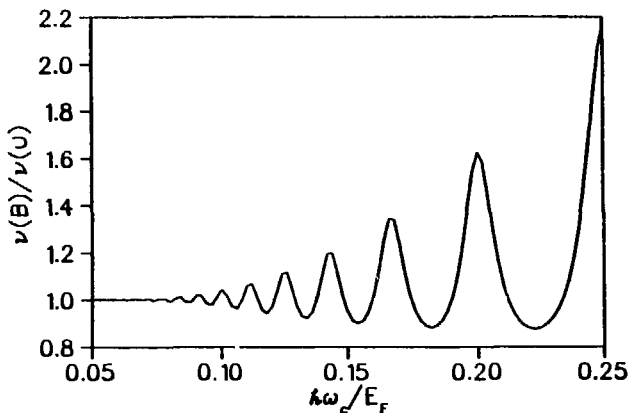


Fig. 1

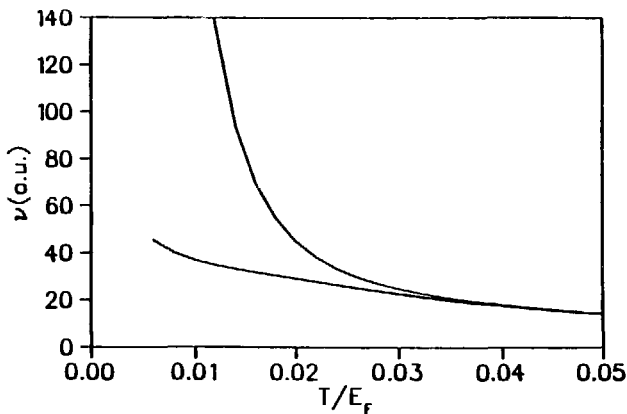


Fig. 2