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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

HOPPING ABSORPTION EDGE IN SILICON INVERSION LAYERS *

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ABSTRACT

The low frequency gap observed in the absorption spectrum of silicon inversion layers is related to the AC variable range hopping. The frequency dependence of the absorption coefficient is calculated.

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Space charge layers have recently been intensively studied. The concentration of the 2D electron gas can be varied over several orders of magnitude of the applied voltage, while the impurities and the interface disorder lead to localization of the electrons in the tails of the surface subbands and form impurity bands. When increasing the concentration, the Fermi level enters the conductive states region, leading to a metal-insulator transition. The microwave and infrared conductivity was studied by Allen, Tsui and De Rosa (1975) in both metallic and localized regimes. The DC conductivity was found to be activated through nearest neighbour hopping with concentration dependent intercept. The high frequency conductivity in the localized regime measured in the 1-40 cm^{-1} range was found to have a low frequency edge centered at the activation energy E_a . Initially this edge was interpreted as a gap in the excitation spectrum due to the strong electron-electron interaction. Adkins (1978) suggested a Wigner glass-gap of the 2D electron gas. A different possibility was considered by Allen, Wilson, Tsui, Gold and Götze (1982).

In this letter the low frequency edge in the microwave absorption is shown to result from hopping between nearest neighbour centers preceding the AC variable range hopping transitions. This mechanism, being in accordance with the DC conductivity behaviour, is a rather general one valid also in 3D materials. An advantage of this conjecture is that it not require gaps in the density of states always situated on the Fermi level, which in quite different materials is unlikely. The frequency dependence of the AC conductivity is calculated here and the role of the temperature and the applied electric field are discussed briefly (see also Kostadinov 1971, 1980).

Let us consider the situation with the Fermi level E_F being placed in the tail of the surface subband produced by the Na^+ ions with concentration of the order of $10^{10} - 10^{12} \text{ cm}^{-2}$. The density of states is illustrated in Fig.1. The activation energy of the DC conductivity at low temperatures depend on the gate voltage V_g . By increasing V_g the Fermi level is pushed towards the surface subband edge and consequently a metal-insulator transition is realized. In fact, the low temperature mobility has a strong power-type temperature dependence, as shown recently by Dean and Pepper (1982), but here the localized regime is considered.

The low frequency absorption results in transitions from one localized level to another one. With increasing frequency the higher level may become eventually delocalized. The probability for such transitions depends on the energy difference of the levels, but in a more crucial manner on the distance R among the centers of localization, being proportional to $\exp(-kR)$ (the simple exponential localization is assumed here though this is not the only possibility)

$$W_{i,f} = 2\pi | \langle i | V | f \rangle |^2 \int \delta(\omega + E_i - E_f) N_i (1 - N_f) \quad (1)$$

Introducing the pair distribution function $P(R, E)$, which is essentially the probability of finding two centers of localization near the Fermi level with level difference E at distance R apart, the transition rate is then found to be proportional to the expression

$$W = \text{const.} \int dR \exp(-2kR) \int dE P(R, E) \delta(E - \omega) \quad (2)$$

where N_i are the occupation numbers of the levels E_i centered at R_i and $P(R, E) = \sum_{\langle i, f \rangle} N_i (1 - N_f) \delta(R - R_{if}) \delta(E + E_i - E_f)$.

Note that $P(R, E)$ is normalized so that

$$\int dE P(R, E) = g(R) \cdot N(E_F)$$

where $g(R)$ is the radial distribution function and $N(E_F)$ is the density of states at the Fermi level. A model of this function was shown to

reproduce well the Mott $T^{-1/4}$ law for the DC variable range hopping conductivity. In this model an average level difference is used

$$E(R) = E_0 \cdot (\bar{R}/R)^3 \quad (3)$$

where E_0 is essentially the nearest neighbour's hopping activation energy and \bar{R} is the mean distance among the localization centers. With $E(R)$ the probability $P(R, E)$ takes the form

$$P(R, E) = N(E_F) \cdot g(R) \cdot \exp(-kR) \quad (4)$$

Using this expression the absorption coefficient is found to be

$$\alpha(\omega) = \text{const.} \exp(-2kR(\omega)) \cdot g(R(\omega)) \quad (5)$$

where the AC variable range hopping distance is determined by the energy conservation

$$\omega = E_0 (\bar{R}/R)^3 \quad (6)$$

For small frequencies $R(\omega) \approx \omega^{-1/3}$, $g(R) = \text{const}$ and the absorption tends to zero exponentially, and that is what was called here hopping absorption edge.

$$\alpha(\omega) \approx \exp(-(\omega_0/\omega)^{1/3}) \quad (7)$$

In the region $\omega = E_0$ the space distance does not vary (nearest-neighbours hopping) and the level difference is also constant. The dependence of the absorption coefficient is due mainly to the radial distribution function. When ω increases the transitions gradually enter the surface subband. The final state for the transition becomes an extended state, which is centered on an infinite cluster. The matrix element of the momentum is written then in the form

$$\langle i | p | f \rangle = \sum_c \exp(-kR_{ic}) \cdot a_c \cdot \langle i | p | c \rangle$$

where the summation is restricted to the nearest neighbours R_c of the localized state, which belong to the infinite cluster of the final state. Using this expression the form (2) of the transition rate is reached, but now $P(R, E)$ is constructed for the localized initial state and the extended final state. The relation (4) is no longer valid, but using it as an ap-

proximation one may expect a structure in the absorption coefficient due to the radial distribution function variations.

In Fig.2 the results of Allen,Wilson,Tsui, Gold and Götze (1982) are shown. The experimentally observed real part of the conductivity decreases rapidly in the low frequency region in accordance with hopping absorption edge suggested here. The behaviour at higher frequencies is described rather qualitatively here, but non-monotonic behaviour is not excluded.

In the case when the Fermi level is sufficiently lowered, the edge is substituted by a peak, whose form is determined by the phonon emission-assisted transitions. Actually, when the photon energy is higher than E_a then hopping transitions to the nearest neighbour centers are possible, the energy excess being dropped as a phonon. For such transitions the space distance is almost constant ($= \bar{r}$) and consequently the momentum matrix element is constant giving rise to constant absorption coefficient. For frequencies much higher than E_a the absorption coefficient decreases as shown by Kostadinov (1980) since the probability of emitting large phonons is decreasing. The temperature dependence of such a broad (of the order of E_a) band is negligible and results in a red shift of the hopping absorption edge of the order of T . Applied electric field increases the band width by energy eFR , which is usually small.

Here it may be worth emphasizing the fact that the variable range hopping leads to a gap in the absorption spectrum, when no such gap is present in the density of states. It is also interesting to find the relation between the non-monotonic behaviour of the absorption and the structure of the impurity radial distribution, since it may serve as a tool.

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FIGURE CAPTIONS

Fig.1 - Density of states in the surface subband tail. Occupied states are shaded.

Fig.2 - Experimental real conductivity in the localized regime. Insert shows $\ln \sigma$ versus $1/T$. (From Allen, Wilson, Tsui, Gold and Götze, 1982.)

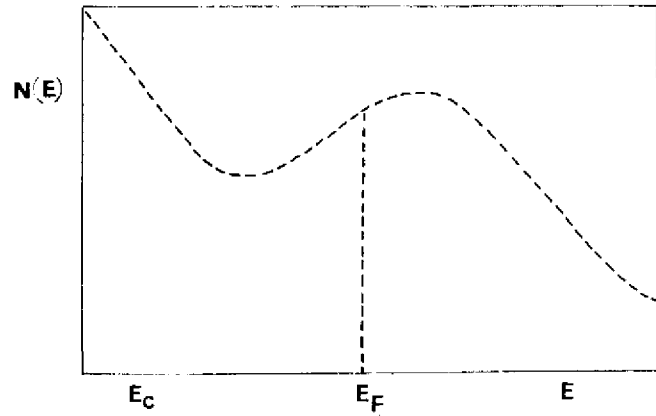


Fig.1

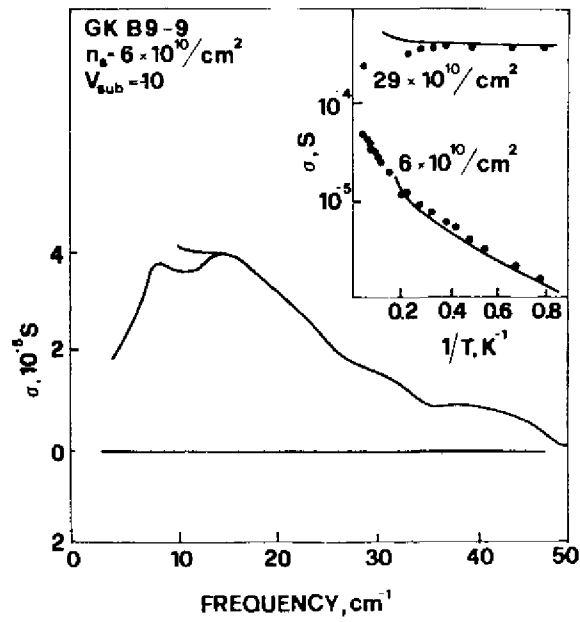


Fig.2



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VARIABLE SCALING METHOD AND STARK EFFECT IN HYDROGEN ATOM *

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ABSTRACT

By relating the Stark effect problem in hydrogen-like atoms to that of the spherical anharmonic oscillator we have found simple formulas for energy eigenvalues for the Stark effect.

Matrix elements have been calculated using $O(2,1)$ algebra technique after Armstrong and then ^{the} variable scaling method has been used to find optimal solutions. Our numerical results are compared with those of Hioe and Yoo and also with the results obtained by Lanczos.

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Some time ago Hioe and Yoo (1983) derived perturbation series for weak and strong field for approximating resonances of the Stark effect.

It was pointed out long ago by Titchmarsh(1958) that a hydrogen atom in the presence of an electric field has no discrete energy eigenvalues. However, the perturbation series is useful if considered as an approximation to a pole of the perturbed Green's function. The poles are interpreted as resonances. The Borel summability of the perturbation series for the resonances of the Stark effect was shown by Graffi and Grecchi (1978) and by Herbst and Simon (1978).

Graffi et al. (1979) showed that the convergence of the diagonal Padé approximants sequence. The method employed by Hioe and Yoo is essentially that of finding the inverse of elliptic integral functions. This method is rather difficult and cumbersome and for strong field one needs many terms.

In this note we relate the problem of ^{the} Stark effect to that of spherical anharmonic oscillator and use the $O(2,1)$ algebra technique after Armstrong (1971) for finding the matrix elements of r^S taken between the three-dimensional harmonic oscillator radial functions. We then use the variable scaling method to find the energy eigenvalues. This method gives simple algebraic equations involving the eigenvalues from which energy eigenvalues are numerically evaluated. Numerically our results agree with those of Hioe and Yoo for weak fields but differ from their results for strong fields, particularly in the case when $n > 1$. But our results are consistent with those of Lanczos.

II. MATHEMATICAL METHODS

The Stark problem can be reduced to that of quartic anharmonic oscillator by the standard method using parabolic coordinates as described in any textbook on quantum mechanics (for example see Fock (1978)). We reproduce here the essential steps. The Schrödinger equation for the hydrogen atom in the presence of an electric field directed along the z axis is

$$\nabla^2 \Psi + 2 \left(E + \frac{1}{r} - \epsilon z \right) \Psi = 0, \quad (1)$$

In writing (1) we have used atomic units. In this unit the electric field intensity is the field produced by a proton at a distance equal to the radius of the first Bohr orbit of hydrogen, viz

$$E/a^2 = 5.142 \times 10^9 \text{ volt/cm} \quad (2)$$

Hence even in very strong field of 10^5 or 10^6 v/cm, G will still be small. Now to solve (1), parabolic coordinates can be used in the following way:

$$\xi = \rho + z, \quad \eta = \rho - z \quad (3)$$

where $\rho^2 = x^2 + y^2$, x, y, z being the Cartesian coordinates.

Then putting $\xi = u^2$, $\eta = v^2$ and assuming a solution of (1) in the form

$$\psi = u^{-1/2} v^{-1/2} e^{im\phi} \chi_1(u) \chi_2(v) \quad (4)$$

equation (1) reduces to two separate equations, viz

$$-\frac{d^2 \chi_1}{du^2} + \left[-2Eu^2 + Eu^4 + \frac{m^2 - 1/4}{u^2} \right] \chi_1 = K \chi_1 \quad (5)$$

and

$$-\frac{d^2 \chi_2}{dv^2} + \left[-2Ev^2 - Ev^4 + \frac{m^2 - 1/4}{v^2} \right] \chi_2 = (K' + 4) \chi_2 \quad (6)$$

with the condition

$$K_{n_1, m} + K'_{n_2, m} = 0 \quad (7)$$

We consider equations (5) and (6) as perturbation problems and use variational analysis to tackle these equations. We describe the procedure for equation (5) and equation (6) can be treated in a similar manner. Using the change of variables

$$u_1 = \omega_0^2 u \quad (8)$$

where $\omega_0^2 = \sqrt{-2E}$ (5) can be written as

$$-\frac{d^2 \chi_1}{du_1^2} + \left[u_1^2 + g u_1^4 + \frac{(m^2 - 1/4)}{u_1^2} \right] \chi_1 = K \chi_1 \quad (9)$$

where

$$g = \frac{E}{\omega_0^2} \quad (10)$$

To solve (9) we use as trial wave functions, spherical harmonic oscillator wave functions of a certain frequency ω and angular momentum ℓ given by $\ell = m - 1/2$.

Now equation (9) can be written as

$$H \chi_1 = K \chi_1 \quad (11)$$

where

$$H = p^2 + u_1^2 + g u_1^4 + \frac{(m^2 - 1/4)}{u_1^2} \quad (12)$$

The trial wave functions $\bar{\chi}$ say satisfies the Schrödinger equation given by the

$$H_0 \bar{\chi} = E_{n_1, \ell} \bar{\chi} \quad (13)$$

where

$$H_0 = p^2 + \omega_0^2 u_1^2 + \frac{(m^2 - 1/4)}{u_1^2} \quad (14)$$

then $E_{n_1, \ell} = 2(2n_1 + m + 1)$

(15)

(the factor 2 appears in equation (5) because of our definition for H_0 (equation (14)). For a variational analysis of the energy K , given in (11), we calculate $\int \bar{\chi}^* H \bar{\chi} d\tau$ and minimize this quantity, subject to the condition $\int \bar{\chi}^* \bar{\chi} d\tau = 1$,

with respect to ω (Epstein (1974), Moshinsky (1969)). Some time ago Armstrong (1971) calculated the matrix elements of r^s taken between eigenstates of spherical anharmonic oscillator. Armstrong used the results of $O(2,1)$ algebra to calculate these matrix elements. Using the same technique the matrix elements $\int \bar{\chi}^* H \bar{\chi} dt$, can be calculated easily.

The general result is given by

$$\int_0^\infty u^\lambda \bar{\chi}_{n_1, m}^+(u) \bar{\chi}_{n_2, m}^-(u) du$$

$$= \omega^{-\lambda/2} (-1)^{\frac{n_1 - n_2}{2}} \Gamma(m+1 + \lambda/2)^s$$

$$\times \left(\frac{\Gamma[\frac{1}{2}(n_2 + m - \lambda/2) + 1] [\frac{1}{2}(n_1 - m - \lambda/2)]! [\frac{1}{2}(n_2 - m - \lambda/2)]!}{\Gamma[\frac{1}{2}(n_1 + m - \lambda/2) + 1]} \right)^{\lambda/2}$$

$$\times \sum_t \frac{(-1)^t}{[\frac{1}{2}(n_1 - m - \lambda/2) - t]! [\frac{1}{2}(2m + n_2 - n_1) + t + 1]!} \left(\frac{\lambda/2}{\frac{n_2 - n_1}{2} + t} \right)^s$$

$$\times \left(\frac{n_1 - n_2 - \lambda - 2}{2} + t \right), \quad (17)$$

where the selection rules are such that when $|n_2 - n_1|$ and s are both odd integers and if $s + 2 > 0$, $n_2 - n_1, s + 2 > 0$

or $n_1 - n_2 \geq s + 2 > 0$

or if $s + 2 \leq 0$, $|n_1 - n_2| \leq -s - 2 < 0$

then the integral must be set equal to zero. Using (17) we get, taking $\kappa_{n_1, m}$ as the

value of the diagonal elements of H ,

$$\kappa_{n_1, m} = \omega (2n_1 + m + 1) + \frac{(2n_1 + m + 1)}{\omega} +$$

$$+ \frac{g}{\omega^2} [(m+2)(m+1) + 6n_1(m+2) + 3n_1(2n_1 - 1)] \quad (18)$$

ω is determined by the condition that $\kappa_{n_1, m}$ should be minimum, viz,

$$\frac{\partial \kappa_{n_1, m}}{\partial \omega} = 0 \quad (19)$$

(19) with (18) give

$$\omega^3 - \omega = \frac{2g [(m+2)(m+1) + 6n_1(m+2) + 3n_1(2n_1 - 1)]}{(2n_1 + m + 1)} \quad (20)$$

A similar analysis can be done for equation (6). Here we just give the results.

$$\kappa'_{n_1, m} + 4/\omega_1^2 = \omega' (2n_2 + m + 1) + \frac{(2n_2 + m + 1)}{\omega'}$$

$$- \frac{g}{\omega_1^2} \frac{[(m+2)(m+1) + 6n_2(m+2) + 3n_2(2n_2 - 1)]}{(2n_2 + m + 1)}, \quad (21)$$

where ω_1 satisfies the equation

$$\omega_1^3 - \omega_1 = \frac{-2g' [(m+2)(m+1) + 6n_2(m+2) + 3n_2(2n_2 - 1)]}{(2n_2 + m + 1)} \quad (22)$$

Equations (18) to (22), together with the condition $\kappa_{n_1, m} + \kappa'_{n_2, m} = 0$, give three simultaneous equations for ω, ω' and ω_0^2 . Solving them we get ω_0^2 and hence E . For small ϵ , these equations can be solved by the following procedure. For the sake of simplicity, let us consider the case, $n_1 = n_2 = 0$. Then (18) to (22) reduce to

$$\omega^2 - \omega - 4g = 0 \quad (23)$$

$$\omega'^3 - \omega' + 4g = 0 \quad (24)$$

and

$$\omega + 1/\omega + \omega' + 1/\omega' + 2g(\omega^2 - 1/\omega^2) - 4/\omega_0^2 = 0 \quad (25)$$

Assume, $\omega = 1 + \epsilon, \omega' = 1 - \epsilon, \omega_0^2 = x$ then it can be easily seen that x satisfies the equation

$$x^6 - x^5 + 2\epsilon^2 = 0 \quad (26)$$

Equation (26) can be solved numerically for x using Newton-Raphson's method, for a given ϵ .

III. SECOND ORDER CORRECTION

The second order correction to $\kappa_{n_1, m}$ and $\kappa'_{n_2, m}$ denoted by

$$K_{n_1, m}^{(2)} = \frac{\sum_p \langle n_1 | -(1+\omega^2)u_1^2 + gu_1^4 | p \rangle^2}{K_{n_1, m}^0 - K_{n_1+p, m}^0} \quad (27)$$

and

$$K'_{n_2, m}^{(2)} = \frac{\sum_p \langle n_2 | -(1+\omega'^2)\omega_1^2 - g\omega_1^4 | p \rangle^2}{K'_{n_2, m}^0 - K'_{n_2+p, m}^0} \quad (28)$$

where $\kappa_{n_1, m}^0$ and $\kappa'_{n_2, m}^0$ are given by equations (18) and (21), can easily be calculated using the technique of $O(2,1)$ algebra (Armstrong (1971)). For the particular case, $n_1 = n_2 = 0, m = 0$, the energy equation up to second order is given by

$$\omega + 1/\omega + \omega' + 1/\omega' + 2g(\omega^2 - 1/\omega^2) + \frac{4g^2}{\omega^4 \left(\frac{\kappa_{0,0}^0}{\omega_0^2} - \frac{\kappa'_{4,0}^0}{\omega_0^2} \right)} + \frac{4g^2}{\omega^4 \left(\frac{\kappa'_{0,0}^0}{\omega_0^2} - \frac{\kappa_{4,0}^0}{\omega_0^2} \right)} - 4/\omega_0^2 = 0 \quad (29)$$

IV. RESULTS AND DISCUSSIONS

Instead of giving the values of E directly we compute the quantity $-2(E-E_0)/\epsilon^2$, for the case $n_1 = n_2 = 0$, and $(E-E_0)/\epsilon$ otherwise.

In Table 1 we compare our values of $-2(E-E_0)/\epsilon^2$ with those obtained by Hioe and Yoo for $n_1 = n_2 = m = 0$. It is seen that for $\epsilon > 16 \times 10^{-3}$ our results differ from those of Hioe et al. It seems that the fourth-order corrections are not negligible for such values of electric field intensity. To see the fourth order effect, we assume

$$-2(E-E_0)/\epsilon^2 = 4.25 + A\epsilon^2 \quad (30)$$

and compute s from the approximate formula given by Lanczos (1931). Though Lanczos' results are very accurate only for $n > 1$, we use this formula to guess the order of magnitude of the fourth order corrections. We give the numerical results obtained from formula (30). Considering the fact that for $n_1 = n_2 = 0$, Lanczos' result would underestimate s , our results are not inconsistent with his results. In Table 2 we compare the values of $(E-E_0)/\epsilon$. Column (2) gives the results of Hioe et al. Column (3) gives those obtained from 3rd order formulas (Bethe and Salpeter (1957)). Column (4) gives the results of the present work. Lastly, column (5) gives the results computed from Lanczos' fourth order formula (Lanczos (1931), equation (66)).

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It seems that for $n_1 = 10$, $n_2 = 0$, fourth order effect is significant even for moderate field strength of the order of 10^4 v/cm.

Thus our results agree with those of Hioe et al. for weak fields and where fourth order effects are significant our results are consistent with those of Lanczos.

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TABLE 1

$$\Delta = -2(E - E_0)/\epsilon$$

ϵ	Δ (Hioe et al.)	Δ (present)	Δ (Lanczos)
.016	4.25	4.25	4.25
.032	4.25	4.27	4.26
.048	4.25	4.29	4.27
.06	-	4.44	4.29

TABLE 2

$$\Delta_1 = (E - E_0)/\epsilon$$

ϵ	Δ_1 (H)	Δ_1 (BZS)	Δ_1 (P)	Δ_1 (L)
6.4×10^{-6}	156.3	156.6	159.4	156.6
8×10^{-6}	154.3	155.2	157.0	155.0
16×10^{-6}	145.9	151.7	145.8	150.0