Polaronic aspects of two-dimensional electrons on films of liquid He

S. A. Jackson and P. M. Platzman
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 4 May 1981)

We have formulated the problem of two-dimensional electrons on a film of liquid helium as a polaron problem and have used the Feynman formulation of the polaron to compute the ground-state energy and the effective mass of the system for all values of the coupling constant (from strong to weak). We find that the effective mass undergoes an extremely rapid transition from an electronic value to a value on the order of several helium-atom masses for coupling constants which are easily attainable; i.e., a "localization" transition occurs.

By now it is well known that image potential bound electrons at the surface of liquid helium are essentially two dimensional (2D); i.e., the energy level spacing for motion perpendicular to the surface is typically large compared to the temperature so that (at helium temperatures) there is no motion in this direction, and attention can be focused on the in-plane dynamics of the carriers.[1] The motion in the plane of a single electron is free except for coupling to the thermally excited ripples of the liquid surface. This coupling is particularly simple and directly analogous to electron-phonon coupling in 3D crystals. The interaction between electrons and ripplons comes about because of the change in energy of the electron as it rides on the surface waves in the presence of an electric field $\mathcal{E}$ (image plus external).

The one-electron properties of this ideal system are of interest because of the variability of the coupling to the ripplons. The use of different substrates for the liquid-helium film or of different film thicknesses allows a change in the effective coupling over several orders of magnitude.[2] For bulk helium (zero external field), $\mathcal{E} \simeq 10^2$ V/cm, and the electron-ripplon coupling is weak. As the helium thickness is reduced to 100 Å, large image potential fields contribute to the total field which increases to $\mathcal{E} \simeq 10^5$ V/cm. At these fields the electron-ripplon coupling is strong and new interesting nonperturbative polaronic effects may occur.

Sander[3] has already published what amounts to a strong-coupling calculation of the ground-state energy of this system. He has shown that the ground state for a sufficiently thin film consists of an electron trapped in a dimple whose size is roughly the capillary length ($\lambda_c = k_c^{-1}$, for 100-Å films $\lambda_c \cong 100$ Å), and the binding energy is about 10 K. In this Communication we will investigate a few of the polaronic properties of this system. More precisely, we will use the Feynman[4] formulation of the polaron to compute the ground-state energy and effective mass of the system. We will be able to show that the mass of this polaron undergoes an extremely rapid "transition" from an electronic value to a value on the order of several He atom masses for coupling constants (electric field, film thickness) which are easily attainable. Some speculations about possible temperature dependence will also be made.

The interaction of electrons of mass m with ripplons of frequency $\omega_{\vec{k}}$ can be described by the polaron Hamiltonian

$$H = \frac{p^2}{2m} + \sum_{\vec{k}} a^{\dagger}_{\vec{k}} a_{\vec{k}} \hbar\omega_{\vec{k}} + U \quad . \tag{1}$$

When there is a strong electric field present the interaction potential $U = e\vec{\mathcal{E}} \cdot \vec{\delta}$ with $\vec{\delta}$ the displacement of the surface. Expanding $\vec{\delta}$ in ripplon modes yields

$$U = \frac{1}{A^{1/2}} \sum_{\vec{k}} (a_{\vec{k}} + a^{\dagger}_{\vec{k}}) e^{i\vec{k}\cdot\vec{r}} Q(k) \tag{2}$$

with

$$Q(k) = \left(\frac{hk \tanh kd}{2\rho\omega_{\vec{k}}} \right)^{1/2} e\mathcal{E} \quad . \tag{3}$$

Equation (2) is valid whenever the distortion of the helium surface is small compared to d and the forces from the image charge in the substrate dominate the forces arising from polarization of the helium. These two conditions certainly are well satisfied for $10 < d < 10^3$ Å. In this case

$$\mathcal{E} = \frac{e^2}{4d^2} \left(\frac{\epsilon - 1}{\epsilon + 1} \right) + \mathcal{E}_{\text{ext}}$$

for a substrate of dielectric constant ϵ. The ripplon frequency for such films $d \simeq 100$ Å, is given by the hydrodynamic equation,[2]

$$\omega_k = [(g'k + \sigma k^3/\rho) \tanh kd]^{1/2} \quad , \tag{4}$$

where ρ, σ, and g' are, respectively, the density, surface tension, and acceleration of the fluid due to its van der Waals coupling to the substrate. For real

substrate materials and for $d \simeq 100$ Å, $g'/g \simeq 10^8$ (g being the acceleration due to gravity) and the capillary constant $k_c = (\rho g'/\sigma)^{1/2} = 6 \times 10^5$ cm^{-1}.

Without going into any real detail it suffices to say that the Feynman[4] method consists of eliminating the phonon coordinates from the problem in favor of a retarded interaction of the electron with itself. The resulting functional integral for the energy, being intractable, is replaced by a simple exactly solvable quadratic functional. Since the first term in the perturbation expansion (in the difference between the two actions) is an upper bound to the energy, the parameters in the approximate action may be determined by minimizing the energy. The so-called two-parameter model assumes that the electron interacts with a single particle of mass M via a spring with spring constant κ. The Lagrangian characterizing this interaction is

$$L = \tfrac{1}{2} m \frac{d\vec{x}^2}{dt} + \tfrac{1}{2} M \frac{d\vec{y}^2}{dt} - \tfrac{1}{2}\kappa(\vec{x}-\vec{y})^2 \ , \qquad (5)$$

where $\vec{x}$ is the 2D coordinate of the electron, and $\vec{y}$ is the 2D coordinate of the fictitious particle. The two parameters v and w defined in terms of κ and M, i.e., $\kappa/m = (v^2 - w^2)$ and $M/m = (v^2 - w^2)/w^2$ are a more conventional choice. A simple normal mode analysis of the Lagrangian shows that v is the internal frequency of relative motion and that $v^2/w^2 = (M+m)/m$ is the total mass of the composite system.

The trial energy of the system in this two-parameter model is given by

$$E = \frac{1}{2}\frac{(v-w)^2}{v} - A \ , \qquad (6)$$

where (in the appropriate units $m = \hbar = 1$)

$$A = \int d\tau \int \frac{d^2k}{(2\pi)^2} |Q(k)|^2 e^{-\omega_k \tau} e^{-(k^2/2)F(\tau)} \ . \qquad (7)$$

In Eq. (7),

$$F(\tau) = \frac{v^2 - w^2}{v^3}(1 - e^{-v\tau}) + \frac{w^2}{v^2}\tau \qquad (8)$$

is the time-dependent response function of the two-oscillator system described by Eq. (5), and $Q(k)$ is the coupling constant given in Eq. (3).

Because of the form of the phonon dispersion and the complexity of the coupling $Q(k)$ the evaluation of the integrals except at strong coupling must be done numerically. However, we have found by a careful examination of the analytic form and numerical results for ($d \simeq 100$ Å) that the problem is well approximated by assuming $\tanh kd \simeq kd$ and,

$$\omega_k = sk, \quad s = (g'd)^{1/2}, \quad k < k_c \ . \qquad (9)$$

In this cutoff approximation the integrals over k and τ may be performed analytically in the strong-coupling and weak-coupling limits.

Let us define a coupling constant $\alpha \equiv (e\mathcal{E})^2/[8\pi\sigma(\hbar^2 k_c^2/2m)]$; energy in units of $k_c^2/2$.[5] In the strong-coupling limit ($\alpha \to \infty$) $v \sim \alpha^{1/2}$, $w/v \to 0$, and $F(\tau) \simeq 1/v$. Thus,

$$E = \tfrac{1}{2}v - \alpha v(1 - e^{-1/v}) \qquad (10)$$

minimizing with respect to v yields $v = \alpha^{1/2}$ and

$$E = -\alpha + \sqrt{\alpha} + \cdots \ ; \qquad (11)$$

i.e., the strong-coupling limit [$F(\tau) = 1/v$] gives a power series in $\sqrt{\alpha}$. It is important to point out that there is no minimum for $\alpha < \frac{1}{2}$. This is true because the range of the strong-coupling effective potential is short and a critical value of the coupling constant is needed to bind an electron in its well. The corrections due to the time dependence of $F(\tau) \simeq 1/v + w^2/v^2\tau + (1/v)e^{-v\tau}$ arise from two physically distinct effects: recoil ($w^2\tau/v^2$) and internal excited states [$(1/v)e^{-v\tau}$]. A minimization of the energy including these two terms to lowest order shows that another physically relevant parameter $\eta \equiv \omega_c/(k_c^2/2)$ comes in. (For 100-Å films $\eta \simeq 5 \times 10^{-3}$.) The energy

$$E_{sc} = (-\alpha + \alpha^{1/2} + \cdots) - \frac{19}{40}\eta - \frac{9}{16}\frac{\eta^2}{\alpha^{1/2}} + \cdots \ . \qquad (12)$$

The term in parentheses is identical to Eq. (11) and comes from setting $F(\tau) = 1/v$. The term linear in η comes from corrections due to the internal excitations energy, i.e., $e^{-v\tau}$, and the η^2 term comes from the recoil of the entire object.

In the weak-coupling regime $v/w \to 1$; i.e., $v/w \equiv 1 + \epsilon$. To order ϵ

$$F(\tau) = \frac{w^2}{v^2}\tau + \frac{2\epsilon}{v}(1 - e^{-v\tau}) \qquad (13)$$

and

$$E_{wc} = -(\alpha\eta) - \frac{\pi^2}{2}(\alpha\eta)^2 + \cdots \ . \qquad (14)$$

Thus the weak-coupling expansion ($\eta \simeq 10^{-3}$) appears to be valid for $\alpha \gg 1$.[6] However, we know from our strong-coupling results that the system will essentially switch from a quasifree object to a self-trapped object at $\alpha \sim 1$.

The numerical results for the energy are displayed along with the approximate strong- and weak-coupling results in Fig. 1. The sharp change at $\alpha \simeq 1/2$ is evident. When the polaron is weakly coupled, it is delocalized, and we expect that its mass will be of order 1. When it is strongly coupled, it is localized, and its mass will be of order 10^4 (several helium-atom masses). Since the transition in coupling constant is extremely rapid, we would expect an even more dramatic variation of the effective mass. In Fig. 2 we plot the model mass $m_0 = v^2/w^2$ and

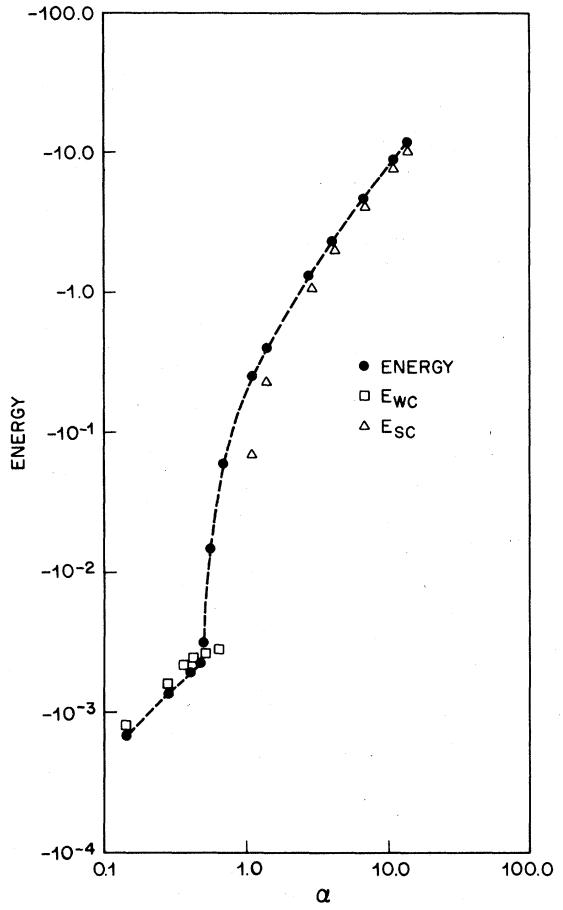

FIG. 1. Energy in units of $\hbar^2 k_c^2/2m$ vs coupling constant α. Points are numerical results; lines are guides to the eye.

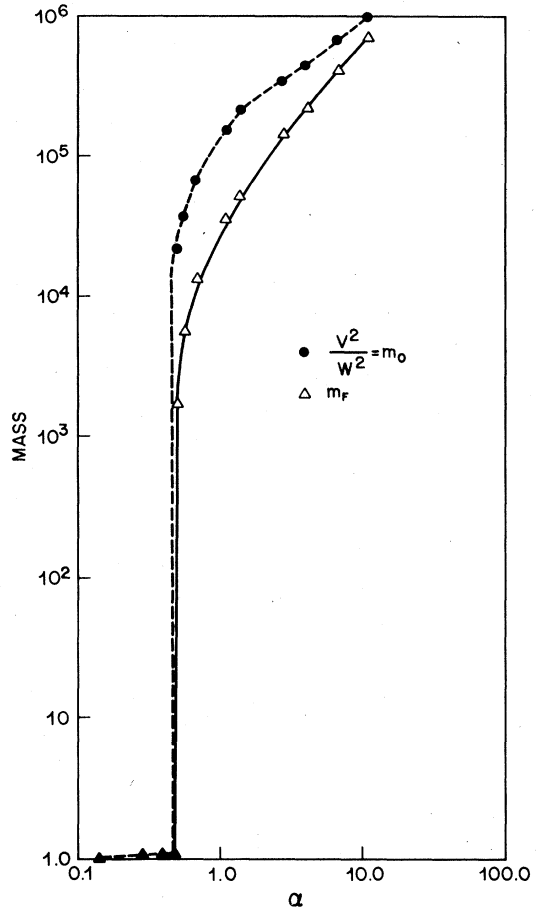

FIG. 2. Model mass (m_0) vs coupling constant α. Feynman mass (m_F) vs coupling constant α. Mass in units of free-electron mass. Points are numerical results; lines are guides to the eye.

the so-called Feynman mass (which comes from calculating the energy as a function of velocity),[4]

$$m_F = 1 + \frac{(e\mathcal{E})^2 d}{8\pi\rho s} \int dq q^4 \int d\tau \tau^2 e^{-\omega_q \tau} e^{-q^2/2F(\tau)} \tag{15}$$

The strikingly rapid four-orders-of-magnitude change in this quantity for a 10% change in α is evident.

We have shown that the existence of a "localization" transition in an ideal system which is, nonetheless, physically realizable. Such a rapid transition from a quasi-free to a quasi-localized state has been speculated on previously for deformation potential systems by Toyozawa and Shinozaka[7] and others.[6,8] We refer to the transition as "localization" because of the rapidity and the size of the change in the effective mass over a very narrow range of coupling constant (<10%). This implies that in a mobility measurement, the diffusion constant would decrease very rapidly. In fact, in the strong-coupling limit, the model mass is proportional to α/η^2. As $\eta \to 0$, this mass $\to \infty$ and the magnitude of the jump in mass at the transition becomes larger for a given value of the coupling constant. Therefore, the transition looks more and more like a real localization transition.

The beauty of the present system is threefold. First, the system corresponds very closely to our continuum electron-phonon model. Secondly, the value of the coupling constant where the transition occurs is in a physically accessible region. Finally, the coupling constant is variable by changing the substrate or by changing the film thickness in the presence of an applied field.

The calculations have assumed a single electron at zero temperature. The validity of these assumptions will depend on the experimental conditions. The scale of the energy $\hbar^2 k_c^2/2m$ for $d \simeq 100$ Å is for the strongly coupled state 10 K. Therefore, we would expect our model to be valid for $n < 10^8$; i.e., the interparticle Coulomb energy $V_C \equiv (e^2/\epsilon^2) n^{1/2} \simeq 1$ K ($n = 10^8$), and for $T < 1$ K.[9]

ACKNOWLEDGMENTS

We would like to thank G. Whitfield for several informative discussions on polarons. We would also especially like to thank B. C. Chambers and A. L. Simons for much help with the numerical aspects of the problem.

---

[1]C. C. Grimes, Surf. Sci. 73, 379 (1978); V. Shikin, *ibid.* 73, 396 (1978).

[2]H. Ikezi and P. M. Platzman, Phys. Rev. B 23, 1145 (1980).

[3]L. M. Sander, Phys. Rev. B 11, 4350 (1975).

[4]R. P. Feynman, Phys. Rev. 97, 660 (1955).

[5]In our calculations we will assume that the coupling constant α is variable. In a real physical system in the absence of an external field it is independent of thickness d and only depends on the dielectric constant of the substrate. For silica $\epsilon = 4$ and $\alpha \simeq 2$. For a variety of substrates $0.01 < \alpha < 10$.

[6]A similar result was found in three dimensions by G. Whitfield and P. B Shaw, Phys. Rev. B 21, 4349 (1980).

[7]Y. Toyazawa and Y. Shinozaka, ISSP Technical Report, Ser. A, No. 992, 1979 (unpublished).

[8]D. Emin and T. Holstein, Phys. Rev. Lett. 36, 323 (1976).

[9]Epsilon appears in the denominator because of the image charge present in the dielectric substrate. For $\epsilon = \infty$ (metal) the law of force between electrons goes over to dipolar.