Detrapping aspects of ripplonic polarons on a liquid helium film

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The problem of two-dimensional electron detrapping from the polaron to the quasifree state above a liquid helium film is studied employing the actual dispersion form of media vibrations. In contrast with the frequently used cutoff approximation, the actual form is shown to result in continuous and quite smooth changes of the polaron energy and mass near the detrapping point. At the same time, the electron localization radius (L) is found to increase rapidly, when the coupling constant ($\alpha_{\rm CC}$) approaches unity: $L\propto(\alpha_{\rm CC}-1)^{-1/2}\to\infty$. In the framework of the general stability analysis, this electron detrapping is explained to be a result of an interesting relationship between the stability index and $\alpha_{\rm CC}$ for the media excitations involved in the polaron cloud.

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The problem of the electron self-trapping to the media vibration cloud has been attracting broad interest for a long while.[1–3] The particularly intriguing question discussed intensively is whether the electron self-trapping occurs continuously or discontinuously when varying the coupling constant $\alpha_{\rm CC}$, characterizing the strength of electron interaction with media vibrations. In other words, is there any critical behavior of the major electron properties at a certain, finite value of the coupling constant $\alpha^*_{\rm CC}$, which can be considered as a sort of phase transition? For the standard Fröhlich system of the free optical polaron, in the framework of an analytical approach, it was shown that such phase transition does not exist.[4] For acoustical polarons, some localization criteria were reported.[5–7] These criteria were formulated in terms of the stability index, which is a combination of the dimension index D, the media dispersion index ν ($\omega_q\propto q^\nu$), and the force range index λ ($g_q=\sqrt{\hbar/2\mu_q\omega_q}V_q\propto q^{-\lambda}$, here V_q is the electron-media coupling, and μ_q is an inertia quantity of the media vibrations). In this treatment, there is a marginal stability index value which separates self-trapped and free electron states. Because the stability index is usually a fixed intrinsic property of a system or a theoretical model (independent of $\alpha_{\rm CC}$), the self-trapping (or detrapping) cannot appear as a result of varying the coupling constant $\alpha_{\rm CC}$, with the exception of the marginal stability index case.

When analyzing the polaron problem in the framework of the Feynman path-integral method for surface electrons formed on a liquid helium film, Jackson and Platzman[8] found that the electron effective mass remarkably underwent an extremely rapid transition from the free-electron value to a much larger value, which was ascribed to the ''localization'' transition. In the variational analysis of Ref. 6, this model ($D=2$, $\nu=1$, and $\lambda=-1/2$) was shown to correspond to the marginal value of the stability index $\delta=D-\nu-2\lambda-2=0$. In this case, the kinetic and interaction terms of the polaron energy have the same dependence on the electron localization radius L, and the total energy $\mathcal{E}_p$, as a function of the coupling constant, changes the sign at $\alpha_{\rm CC}=\alpha^*_{\rm CC}$:

$$\mathcal{E}_p\propto\frac{(\alpha^*_{\rm CC}-\alpha_{\rm CC})}{L^2}. \tag{1}$$

The critical value $\alpha^*_{\rm CC}$ separates the free-electron ($L\to\infty$) and shrunk ($L\to0$) states. In another analysis[7] based on the symmetry arguments, a substantially different stability index

$$\sigma=\frac{D+2-2\lambda}{\nu} \tag{2}$$

was introduced, and the ground state was shown to be delocalized for arbitrary coupling strength if $\sigma>2$. The application of this criterion to the 2D electron system formed on the helium film yields $\sigma=5>2$, which precludes any ''localization'' transition.[7]

First, it should be noted that the abovementioned analysis of Refs. 6 and 7 does not really correspond to the model used by Jackson and Platzman in the full extent. The model employed in the ripplonic polaron treatment is actually a cutoff model which assumes that there are no media excitations with $q>q_c=\kappa$ (here κ is the capillary constant for the surface excitations of the helium film). We shall see that this wave-number cutoff is the most important assumption of the model, which actually introduces the ''localization'' transition for the acoustical polarons. Briefly, this conclusion follows from the fact that κ, combined with the localization radius of the strong coupling limit L_0, relates directly to the polaron coupling constant $\alpha_{\rm CC}=2/\kappa^2L_0^2$ which we shall define later. Thus the cutoff dispersion model of the media vibrations involved in the polaron cloud ($qL_0\sim1$) becomes somewhat dependent on the coupling constant, which appears to be crucial for the self-trapping transition.

Secondly, the cutoff model of the media vibrations does not really reflect the actual excitation spectrum of the liquid helium film, which has no cutoff at $q\sim\kappa$

$$\omega_q=\left[\frac{\alpha}{\rho}(q^2+\kappa^2)q\tanh(qd)\right]^{1/2}\simeq\omega_0\tilde{q}\sqrt{1+\tilde{q}^2}, \tag{3}$$

where α is the surface tension, ρ is the liquid helium mass density, d is the film thickness, $\kappa=\sqrt{\rho G_d/\alpha}$ is the capillary constant, $G_d\propto d^{-4}$ is the acceleration of fluid atoms due to the van der Waals forces, $\tilde{q}=q/\kappa$, and $\omega_0=\sqrt{\alpha d/\rho}\kappa^2$. At $q\sim\kappa$, the dispersion curve just bends and the dispersion index changes smoothly from $\nu=1$ ($q\ll\kappa$) to $\nu=2$ ($q\gg\kappa$; we

consider $qd \ll 1$). Ripplonic polarons with this form of the media vibration spectrum were studied in the framework of the path-integral method by Hipólito, Farias, and Studart[9] and, for the strong coupling regime, by Saitoh.[10] The numerical graphs of the polaron mass, energy, and mobility vs the film thickness d presented in Refs. 9 and 11 show only continuous changes. Still, as noted by Jackson and Platzman, the coupling constant for the ripplonic polaron on the typical helium film is practically independent of d, and therefore it is difficult to reach the detrapping transition by varying the film thickness.

It is of obvious interest to investigate the behavior of the polaron radius L, energy, and mass as functions of α_{CC} for the actual form of Eq. (3). Is there any finite critical value of the coupling constant $\alpha_{CC}^{*}>0$, which can be considered as a bound for the self-trapped states, or the polaron properties vary smoothly down to $\alpha_{CC}=0$? If the detrapping transition exists, how does it relate to the stability criteria found previously in Refs. 6 and 7? In this paper we report the answers to these questions. We found that the polaron bound $\alpha_{CC}^{*}=1$ and detrapping transition exist for the actual ripplon spectrum: in the vicinity of $\alpha_{CC}=1$, a small decrease of the coupling constant causes a huge increase of the electron localization radius, and $L\to\infty$ when $\alpha_{CC}\to 1$. Nevertheless, the polaron energy and mass are continuous and quite smooth functions of the coupling constant. The sharpness or the steplike behavior of the polaron mass reported previously[8] is shown to be a result of the cutoff approximation. The detrapping transition appears because the dimensionless parameter $\tilde{q}^2=(q/\kappa)^2$, entering Eq. (3), depends on the coupling constant for the wave numbers $q\sim\sqrt{2}/L$ giving the major contribution to the polaron properties: $\tilde{q}^2\sim\alpha_{CC}/l^2$ (here $l=L/L_0$ is the normalized electron localization radius). When the coupling constant passes through the region $\alpha_{CC}\sim 1$, the dispersion index ν of the media vibrations transforms from 2 to 1, affecting crucially the polaron stability index.

It should be emphasized that the media excitation dispersion of Eq. (3) does not depend on the interaction and the coupling constant in the direct way. The indirect dependence on α_{CC} appears because the interaction with a localized electron selects the specific wave-numbers $q\sim\sqrt{2}/L$ giving the major contribution to the polaron energy. Since the localization radius depends on the interaction strength, the dispersion index of the excitations relevant becomes dependent on α_{CC}.

The actual dispersion form of Eq. (3) is more complicated than the acoustical cutoff model. Because the dispersion form is crucial for the detrapping transition, we choose to use the simple adiabatic polaron treatment (similar to that of Ref. 6) with the exact dispersion rather than the more advanced and complicated method with an approximate dispersion. The adiabatic method assumes that an electron is localized in the relative (electron-media excitation cloud) coordinates, and the combined system can move freely with an effective (polaron) mass. In this framework, we can study the behavior of the localization radius L as a function of α_{CC}. If the detrapping transition occurs, one may expect that the localization radius $L\to\infty$ as the coupling constant decreases down to the critical value. Our choice is based also on the fact (shown below) that for the cuttoff model, the conventional adiabatic polaron treatment reproduces the main results of the path-integral method found in Ref. 8.

The ripplonic polaron consists of a self-trapped electron and a surface dimple $\xi(r)$. The latter serves as the media excitation cloud. The analysis of the numerical solution for the electron wave function in the strong coupling limit ($\alpha_{CC}\gg 1$)[11] indicates that it is quite close to a Gaussian form with the localization radius

$$L=L_0\equiv\sqrt{\frac{4\pi\alpha\hbar^2}{m(eE_{\perp}^{*})^2}} \tag{4}$$

found by means of the variational method[12] (here m is the free-electron mass, and $E_{\perp}^{*}$ is the total holding electric field: the external field $E_{\perp}$ plus the image field of the dielectric substrate $E_d\sim d^{-2}$;[13] for thin films, $E_d\gg E_{\perp}$). Therefore it is reasonable to use a Gaussian trial wave function, which yields the following form of the polaron energy:

$$\mathcal{E}_p(L)=\frac{\hbar^2}{2mL^2}-\sum_{\mathbf{q}}\frac{V_q^2}{2\mu_q\omega_q^2}e^{-q^2L^2/2}, \tag{5}$$

where $V_q\simeq eE_{\perp}^{*}$, and $\mu_q=\rho/q\tanh(qd)$. The first term of Eq. (5) is the zero point kinetic energy of the electron, and the second term is the gain of the interaction energy.

There is a certain freedom in definition of the polaron coupling constant α_{CC}. We define it from the condition that the average phonon number of the polaron cloud $\langle N\rangle=\alpha_{CC}$ in the weak coupling regime. Then, the value $\alpha_{CC}=1$ represents the transition regime from weak to strong coupling. This condition yields

$$\alpha_{CC}=\frac{(eE_{\perp})^2}{4\pi\alpha}\frac{2m}{\hbar^2\kappa^2}\equiv\frac{2}{\kappa^2L_0^2}, \tag{6}$$

the value which is exactly two times larger than the notation used previously.[8] The convenience of this choice is that the detrapping transition occurs exactly at $\alpha_{CC}=\alpha_{CC}^{*}=1$.

Before proceeding with the exact dispersion form we would like to show that for the cutoff model, the method employed here reproduces the detrapping transition found previously by means of the path-integral method. First, we note that for the pure acoustical spectrum $\omega_q\propto q$ without the cutoff, Eq. (5) yields the result of Ref. 6: the normalized polaron energy $\tilde{\mathcal{E}}_p=2mL_0^2\mathcal{E}_p/\hbar^2=(1-\alpha_{CC})/l^2$ changes its sign when the coupling constant α_{CC} passes unity, but there is no minimum to fix the normalized localization radius $l=L/L_0$. The situation changes a great deal for the cutoff model of Ref. 8 with $q_c=\kappa$. In this case, the summation over $|q|<\kappa$ yields a different polaron energy equation

$$\tilde{\mathcal{E}}_p=\frac{1}{l^2}[1-\alpha_{CC}(1-e^{-l^2/\alpha_{CC}})]. \tag{7}$$

Here the term $-\exp(-l^2/\alpha_{CC})$, introduced by the cutoff, prevents the electron from shrinking to $l=0$ at $\alpha_{CC}>1$. For $\alpha_{CC}>1$, the polaron energy has a minimum at a finite l,

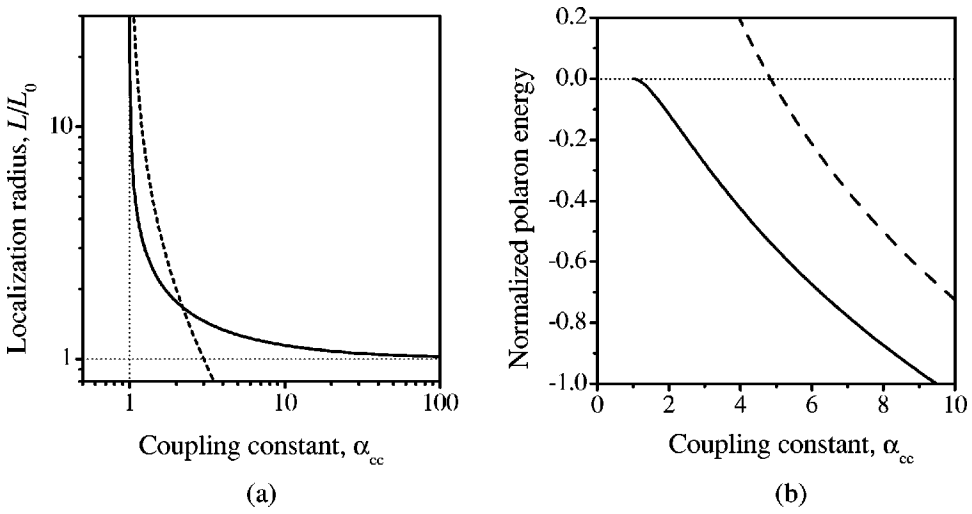

FIG. 1. The normalized electron localization radius $l(\alpha_{CC})$ (a) and polaron energy $\tilde{\mathcal{E}}_p(\alpha_{CC})$ (b) vs the coupling constant: the numerical solution according to Eq. (8) (solid curve), the analytical approximation of Eq. (10) [short-dashed curve, (a)], the strong coupling approximation [dashed curve, (b)].

while at $\alpha_{CC}<1$ there is no minimum. The existence of the detrapping transition of Jackson and Platzman[8] in the conventional adiabatic theory (for the same dispersion model and with the same value of α^*_{CC}) inspires us to apply this method to the actual form of the ripplon dispersion.

Employing the actual ripplon dispersion of Eq. (3), the equation for the polaron radius $\partial\mathcal{E}_p/\partial L=0$ can be written in the following form:

$$\frac{1}{l^2}=\int_0^\infty \frac{x}{x+l^2/\alpha_{CC}}e^{-x}dx. \tag{8}$$

In the region $\alpha_{CC}\gg 1$, the solution of this equation coincides with that of the strong coupling regime $l=1$. This limiting case corresponds to the following stability indexes $\delta=-2<0$ and $\sigma=2$. In the opposite limit $\alpha_{CC}\ll 1$, there is no solution with any finite l. The respective stability indexes are different: $\delta=0$ and $\sigma=5>2$. Therefore for the actual dispersion, the marginal value $\delta=0$ discussed in Ref. 6 is achieved only in the limiting case $l^2/\alpha_{CC}\gg 1$. Thus for Eq. (8), the stability index depends on the coupling constant and, when α_{CC} decreases, it reaches the marginal value, which causes the electron detrapping.

When analyzing Eq. (8) in the region $\alpha_{CC}\sim 1$, it is convenient to represent it as

$$l^2=1+\frac{l^4}{\alpha_{CC}}e^{l^2/\alpha_{CC}}\left[-\mathrm{Ei}\left(-\frac{l^2}{\alpha_{CC}}\right)\right], \tag{9}$$

where $\mathrm{Ei}(x)$ is the exponential-integral function. Expecting a strong increase of $l(\alpha_{CC})$ when $\alpha_{CC}\to\alpha^*_{CC}$, we can use the asymptotical form $\mathrm{Ei}(-x)\simeq -e^{-x}(1/x-1/x^2+2/x^3)$. Such substitution yields the analytical solution

$$l(\alpha_{CC})\simeq\sqrt{\frac{2}{\alpha_{CC}-1}} \tag{10}$$

valid near the critical point for $\alpha_{CC}-1\ll 1$. This solution indicates the existence of the detrapping transition with the same value of α^*_{CC} as that found for the cutoff model. The important difference is that the dependence $l(\alpha_{CC})\propto(\alpha_{CC}-1)^{-1/2}$ is substantially stronger than the logarithmical dependence which can be found for the cutoff model [Eq. (7)].

The numerical solutions of Eq. (8) or Eq. (9) for the electron localization radius $l(\alpha_{CC})$ and the polaron energy are shown in Fig. 1. The critical behavior of $l(\alpha_{CC})$ shown there by the solid curve (a) does not cause any sharp behavior of the polaron energy (b) which changes continuously and smoothly to zero. In the vicinity of the region $\alpha_{CC}=1$, the normalized polaron energy behaves as $\tilde{\mathcal{E}}_p=-(\alpha_{CC}-1)^2/4\to 0$. Another consequence of the numerical graph of Fig. 1(b) is that the polaron energy (solid curve) is always negative, which means that formation of polarons is favorable as soon as $\alpha_{CC}>1$.

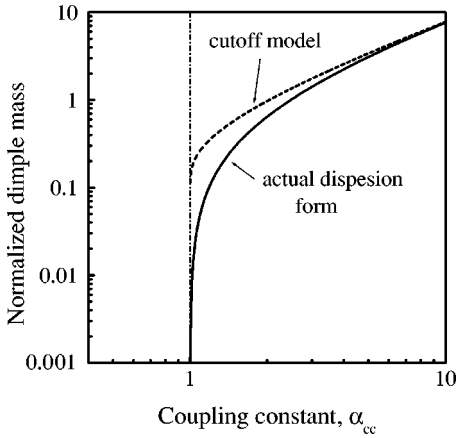

FIG. 2. The normalized dimple mass $M_d/M_d^{(0)}$ as a function of the coupling constant: numerical evaluations of Eqs. (11) and (12) for the actual dispersion form (solid curve) and for the cutoff model discussed in the text (short-dashed curve).

The polaron mass is the sum $M_p = m + M_d$, where M_d is the effective mass of the surface dimple[13]

$$M_d = \frac{\rho}{2} \sum_{\mathbf{q}} (\xi_q)^2 q \coth(qd), \tag{11}$$

$$\xi_q = -\frac{V_q}{\mu_q \omega_q^2} e^{-q^2 L^2/4},$$

and ξ_q is the Fourier transform of the polaron dimple $\xi(r)$. In the limiting case $qd \ll 1$, straightforward evaluations yield

$$\frac{M_d}{M_d^{(0)}} = l^2 \int_0^\infty \frac{e^{-x} dx}{(x + l^2/\alpha_{\mathrm{CC}})^2}, \quad M_d^{(0)} = \frac{\hbar^2 \rho}{4 m \alpha d}. \tag{12}$$

In the strong coupling limit, $M_d \simeq \alpha_{\mathrm{CC}} M_d^{(0)}$.[13] This result was reproduced also in the framework of the Feynman path-integral method.[10,14] Therefore it is reasonable to expect that Eq. (12) will give a quite accurate result in the region $\alpha_{\mathrm{CC}} \sim 1$ as well. For $l \gg 1$, one can find that the dimple mass vanishes smoothly as α_{CC} approaches unity: $M_d \simeq M_d^{(0)} l^{-2} = (\alpha_{\mathrm{CC}} - 1) M_d^{(0)}/2$.

The numerical graph of $M_d(\alpha_{\mathrm{CC}})$ is shown in Fig. 2 by the solid curve. For $d = 100$ Å, we estimate $M_d^{(0)}/m \simeq 1.35 \times 10^5$. The polaron mass indeed changes rapidly from a value of the order of $10^5 - 10^6\, m$ to the free-electron value in a qualitative accordance with the result of Jackson and Platzman. Still, in contrast with the sharp fall of the polaron mass found in Ref. 8, the solid curve of Fig. 2 is smooth. We ascribe the sharpness of that fall to the cutoff approximation. This conclusion follows from the analysis of the cutoff model in the framework of the adiabatic variational method [Eq. (7)]. In this case, the localization radius l increases as $\alpha_{\mathrm{CC}} \to 1$ only with the logarithmical rate. This means that the dimple mass $M_d \simeq M_d^{(0)} l^{-2}$ depends weakly on the difference $\alpha_{\mathrm{CC}} - 1$ as the coupling constant approaches its critical value. Because the polaron energy has no minimum at $\alpha_{\mathrm{CC}} < 1$, and $M_d(\alpha_{\mathrm{CC}})$ is nearly constant at $\alpha_{\mathrm{CC}} > 1$ for the cutoff model, the mass fall, shown in Fig. 2 by the short-dashed curve, really looks similar to a step function. At large values of α_{CC}, the cutoff model surprisingly gives a reasonable result approaching the solid curve, though it deviates strongly from the solid curve at the vicinity of the detrapping point.

In conclusion, we have shown that the detrapping transition of ripplonic polarons on the liquid helium film [$l \propto \sqrt{2/(\alpha_{\mathrm{CC}} - 1)} \to \infty$ as $\alpha_{\mathrm{CC}} \to 1$] originates from the unusual dispersion form of the long-wavelength media vibrations, which represents a very interesting case for the polaron problem. The dispersion and stability indexes for the media vibrations involved in the polaron cloud become dependent on the coupling constant, so that the stability index reaches the marginal value when $\alpha_{\mathrm{CC}} \to 1$. Such situation was not discussed previously in the general stability analysis of the polaron problem. The cutoff model of the media excitation spectrum often used in theoretical studies[8,14] is shown to reflect somehow this feature of the ripplonic polaron, still, at zero temperature, it introduces the too sharp behavior of the polaron mass near the transition point. The actual form of the ripplon dispersion is shown to result in large but smooth and continuous changes of the polaron mass and energy, which agrees with the general analysis of Ref. 7.

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