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Two-dimensional polaron in a magnetic field

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The ground-state energy of a Fröhlich optical polaron confined to two dimensions, placed in a perpendicular magnetic field is calculated within the Feynman path-integral approach. The Feynman-model mass, the magnetization and the susceptibility are calculated as a function of the magnetic field strength for different values of the electron-phonon coupling. We find that within the generalized Feynman approximation the polaron exhibits a discontinuous transition from a dressed state to a stripped state if the electron-phonon constant α is larger than 1.60. For $\alpha < 1.60$, the transition occurs continuously with increasing magnetic field.

I. INTRODUCTION

In the present paper we study the Fröhlich optical polaron in a constant magnetic field which is perpendicular to the plane in which the motion of the electron is confined. This ideal two-dimensional (2D) system has been studied recently by several authors[1–5] in the limit for small electron-phonon interaction. In the present paper we will concentrate on the ground-state property of the 2D polaron system for arbitrary electron-phonon coupling and arbitrary magnetic field strength. We will use Feynman's path-integral approach of the polaron to calculate the ground-state energy, the mass of the Feynman polaron model, the magnetization, and the susceptibility as a function of both the electron-phonon coupling and the magnetic field strength. Results for the Gaussian approximation will also be given. The motivation for using the Feynman approximation lies in the fact that for the three-dimensional (3D) optical polaron in the presence of a magnetic field it was found by two of the present authors that the Feynman path-integral method[6] is superior to all the other existing approaches. For nonzero magnetic field the Feynman approach leads to lower values for the polaron ground-state energy than obtained from other theories. Unfortunately there exists no *mathematical* proof that, in the case of a nonzero magnetic field, the ground-state energy in the Feynman approximation is an upper bound to the exact ground-state energy. But in Appendix A of Ref. 6 strong arguments were given, based on *physical* intuition, in favor of the upper-bound nature of the polaron ground-state energy calculated in the Feynman approximation when a magnetic field is present.

For zero magnetic field the Feynman approximation has been applied to the 2D polaron problem.[7,8] The results show that both ground-state energy and effective mass are continuous functions of the electron-polaron coupling constant α. The same conclusion is true for the 3D optical polaron.[9] However, in Ref. 6 the influence of a magnetic field was examined: the ground-state properties of a 3D polaron were studied and it was found that there exists a transition of the Feynman polaron from a dressed polaron state to a stripped polaron state with increasing magnetic field strength. In the present work we will investigate whether or not a similar magnetic-field-induced transition can be found for the 2D polaron.

The organization of the present paper is as follows. In Sec. II the problem is formulated, the approximations are outlined, and the ground-state energy is calculated. Analytic results for limiting values of α and ω_c are presented and discussed in Sec. III together with our numerical data. The conclusions are presented in Sec. IV.

II. FORMULATION AND APPROXIMATION

The Hamiltonian describing the 2D polaron in a magnetic field is given by[10,11]

$$H=\frac{1}{2m}\left[\mathbf{p}+\frac{e}{c}\mathbf{A}\right]^2+\sum_{\mathbf{k}}\hbar\omega_s a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}}(V_k a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}+V_k^* a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}}) , \tag{1}$$

where $V_k=\hbar\omega_s(\sqrt{2}\pi\alpha/Sk)^{1/2}(\hbar/m\omega_s)^{1/4}$. $\mathbf{p}$ and $\mathbf{r}$ are the electron momentum and positron operators, respectively, $a_{\mathbf{k}}^\dagger$ ($a_{\mathbf{k}}$) is the creation (annihilation) operator of an optical phonon with wave vector $\mathbf{k}$ and energy $\hbar\omega_s$, α is the electron-phonon coupling constant, S is the volume of the 2D crystal, and $\mathbf{A}$ is the vector potential which is taken in the symmetrical gauge: $\mathbf{A}=\frac{1}{2}B(-y,x,0)$.

In the well-known Feynman path-integral representation of the partition function the phonon variables can be eliminated exactly. After this elimination each electron path contributes $e^{-S[\mathbf{r}(t)]}$ to the path integral, with the action

$$S=S_e+S_I , \tag{2}$$

where

$$S_e=\frac{1}{2m}\int_0^\beta du\{\dot{\mathbf{r}}^2(u)+i\omega_c[\dot{y}(u)x(u)-\dot{x}(u)y(u)]\} \tag{3}$$

is the action of a free electron in a magnetic field with $\omega_c = eB/mc$ the cyclotron frequency of the noninteracting electron, $\beta = 1/k_B T$ is the inverse temperature, and

$$S_I = -\sum_{\mathbf{k}} |V_k|^2 \int_0^\beta du \int_0^\beta du' \, G_{\omega_s}(u-u') \times \exp\{i\mathbf{k}\cdot[\mathbf{r}(u)-\mathbf{r}(u')]\} \tag{4}$$

is the action which contains a memory effect as a consequence of the elimination of the phonons. $G_\omega(u) = \frac{1}{2}n(\omega)(e^{\omega|u|}+e^{\omega(\beta-|u|)})$ is the Green's function of the free phonon system with $n(\omega)=(e^{\hbar\beta\omega}-1)^{-1}$ the number of phonons with energy $\hbar\omega$. In the following, for convenience, we will use units such that $\hbar = m = \omega_s = 1$.

Since the path integral with action (2) cannot be solved exactly, we will follow Feynman[12] in order to get an approximation to the exact ground-state energy. For the 3D polaron and in the absence of a magnetic field Feynman introduced a trial action S_0 to derive a variational upper bound to the exact ground-state energy (E_g), i.e., $E_g \le E = E_0 - A - B$, where E_0 is the ground-state energy corresponding to the trial action while A and B are functions which depend on the variational parameters of the trial action S_0. We will use a similar approximation in the present paper. In the case when a magnetic field is present the action is complex and we no longer have a proof that the approximate ground-state energy is an upper bound to the exact polaron ground-state energy. In Ref. 6 intuitive arguments were given which suggest that for a particular choice of the trial action, namely for a trial action derivable from a Hermitian Hamiltonian, the Feynman inequality is still valid.

The trial action we choose is

$$S_0 = S_e + S_{mI} , \tag{5}$$

where

$$S_{mI} = \frac{w(v^2-w^2)}{4} \int_0^\beta du \int_0^\beta du' \, G_w(u-u') \times [\mathbf{r}(u)-\mathbf{r}(u')]^2 \tag{6}$$

and S_e is given by Eq. (3). The action S_0 can be obtained from the Hermitian Hamiltonian (see Ref. 6)

$$H_0 = \frac{1}{2m}\left[\mathbf{p}+\frac{e}{c}\mathbf{A}\right]^2 + \frac{(\mathbf{p}')^2}{2m'} + \frac{1}{2}K(\mathbf{r}-\mathbf{r}') \tag{7}$$

after eliminating the variables of the fictitious particle $(\mathbf{r}',\mathbf{p}')$. Here we have defined the usual Feynman variational parameters v and w. The Hamiltonian H_0 can be diagonalized exactly,

$$H_0 = \sum_{n=1}^{3} s_n (c_n^\dagger c_n + \tfrac{1}{2}) , \tag{8}$$

with the eigenfrequencies s_n to be determined from the solution of the third-order algebraic equation in s_n^2 (for details we refer to Ref. 6)

$$s_n^2(s_n^2-v^2)^2 - \omega_c^2(s_n^2-w^2)^2 = 0 . \tag{9}$$

The variational ground state is then

$$E = \frac{1}{2}\sum_{n=1}^{3} s_n - w - (v^2-w^2)\left[\sum_{n=1}^{3} \frac{s_n d_n^2}{(w+s_n)}\right] - A , \tag{10}$$

where

$$A = \frac{1}{2}\left[\frac{\pi}{2}\right]^{1/2} \alpha \int_0^\infty \frac{e^{-t}}{\sqrt{D(t)}} dt \tag{11}$$

with

$$D(t) = \sum_{n=1}^{3} d_n^2 (1-e^{-s_n t})$$

and

$$d_n^2 = \frac{1}{2s_n} \frac{s_n^2-w^2}{3s_n^2+2(-1)^n s_n \omega_c - v^2} .$$

For $\omega_c \to 0$ Eq. (10) reduced to the familiar result given in Refs. 7 and 8. For given electron-phonon coupling constant α and magnetic field strength ω_c, the parameters v and w are determined by a minimalization of E with respect to v and w.

III. RESULTS AND DISCUSSION

It seems impossible to derived from Eq. (10) an expression in a closed form for the ground-state energy. Only for some limiting values of α and ω_c analytic results can be obtained.

In the small-coupling limit $\alpha \ll 1$ we have $v \approx w$ and the ground-state energy becomes

$$E = \frac{\omega_c}{2} - \frac{\alpha\pi\sqrt{\omega_c}}{2} \frac{\Gamma(1+1/\omega_c)}{\Gamma(\frac{1}{2}+1/\omega_c)} \tag{12}$$

which was recently obtained in Refs. 3 and 5 with second-order perturbation theory. For small magnetic fields $\omega_c \ll 1$, the following series expansion results from Eq. (12):

$$E = \frac{\omega_c}{2} - \frac{\pi\alpha}{2}\left[1+\frac{\omega_c}{8}+\frac{\omega_c^2}{128}+\cdots\right] . \tag{13}$$

In the strong-magnetic-field case we have $(v-w)/v \ll 1$, and consequently we may again start from $v = w$ in Eq. (10). Performing an expansion of Eq. (12) for large ω_c values we obtain the ground-state energy

$$E = \frac{\omega_c}{2} - \frac{\alpha\sqrt{\pi\omega_c}}{2} - \frac{\alpha\sqrt{\pi}\ln 2}{\sqrt{\omega_c}} + \cdots . \tag{14}$$

Note that the electron-phonon correction to the ground-state energy is proportional to $\alpha\sqrt{\omega_c}$ which is much larger than for the 3D case where the correction goes as $\alpha \ln\omega_c$.

For large electron-phonon coupling $\alpha \gg 1$ and weak magnetic fields $\omega_c \ll 1$ we have $v \gg w$ and the ground-state energy, after minimalization with respect to v and w, can be reduced to

$$E = -\frac{\pi}{8}\alpha^2 - 2\ln 2 - \frac{1}{2} + \frac{\omega_c}{2v^2} , \tag{15}$$

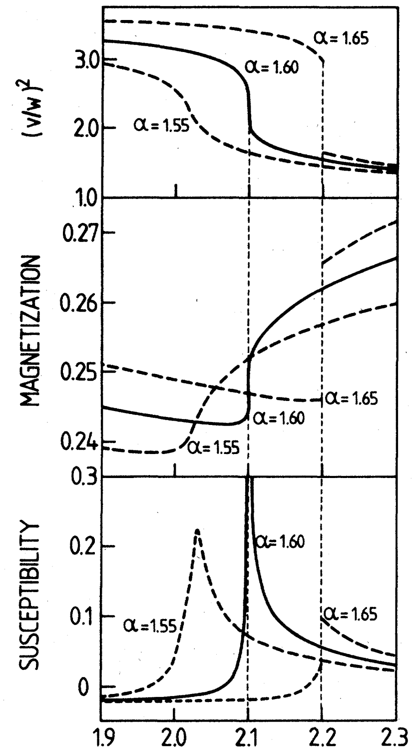

FIG. 1. The mass of the Feynman polaron model, the magnetization, and the susceptibility are shown as functions of ω_c, near the critical point $\alpha \approx 1.60$.

where the variational parameters are given by $w=1$ and $v=(\pi/4)\alpha^2-(4\ln 2-1)$. The terms $-(\pi/8)\alpha^2-2\ln 2-\frac{1}{2}$ are the ground-state energy of a 2D polaron in the strong-coupling limit in the absence of a magnetic field. This result can be obtained directly from the corresponding 3D result by using a scaling argument introduced in Ref. 8. $\omega_c/2v^2$ is the zero-point energy of a particle with mass $v^2=(\pi\alpha^2/4)^2$ placed in a magnetic field.

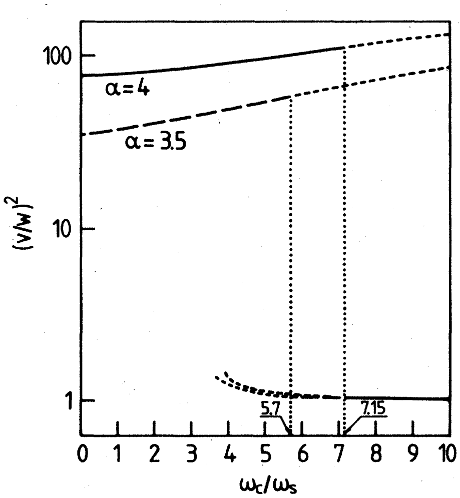

FIG. 2. Feynman polaron mass as a function of ω_c for $\alpha=3.5$ and 4.0.

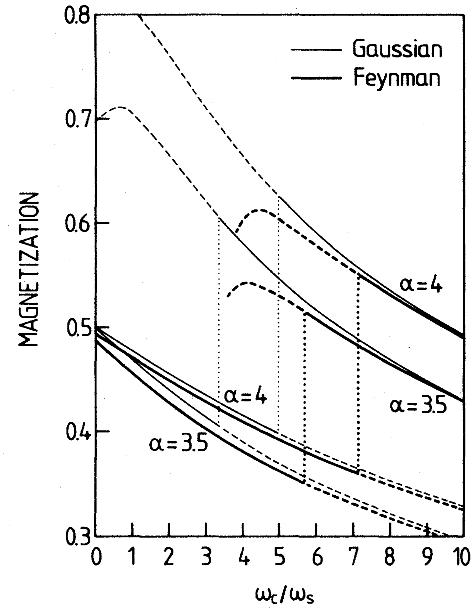

FIG. 3. Magnetization as a function of ω_c for $\alpha=3.5$ and 4.0 in the case of the generalized Feynman approximation (thick solid curve) and for the Gaussian approximation (thin solid curve). Behavior of the metastable state is indicated by the dashed curves.

For arbitrary strength of the electron-phonon coupling constant and the magnetic field the minimalization of E with respect to v and w has been performed numerically. We have calculated numerically the mass of the Feynman polaron model $M=(v/w)^2$, the magnetization $\mu=-\partial E/\partial\omega_c$, and the susceptibility $\chi=-\partial^2 E/\partial\omega_c^2$ for several values of the coupling constant α and the magnet-

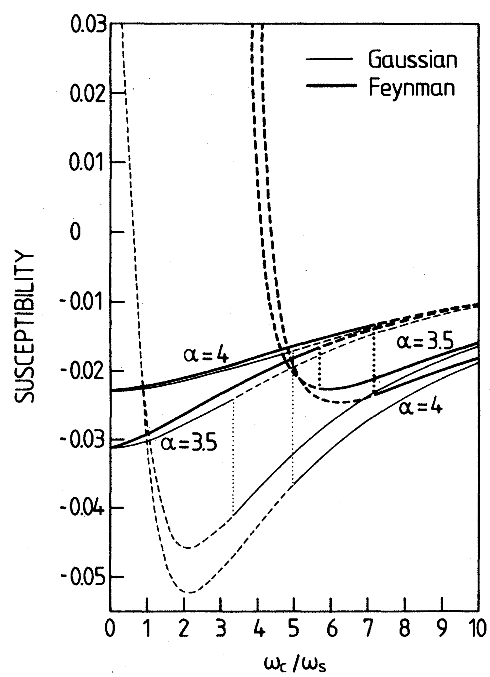

FIG. 4. Same as Fig. 3, but now for the susceptibility.

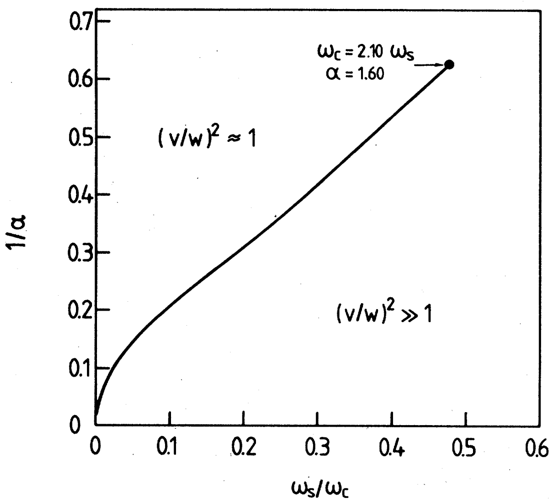

FIG. 5. Phase diagram for the polaron in the generalized Feynman approximation plotted vs the inverse of the electron-phonon coupling strength ($1/\alpha$) and the inverse of the magnetic field strength ($1/\omega_c$).

ic field strength ω_c. In Figs. 1–6, the magnetization $\tilde{\mu}=\mu-\mu_e$ and the susceptibility $\tilde{\chi}=\chi-\chi_e$ are referred to the free-electron values $\mu_e=-0.5$ and $\chi_e=0$. Consequently $\tilde{\mu}$ and $\tilde{\chi}$ are purely a consequence of the electron-phonon interaction.

For $\alpha<1.60$ (see Fig. 1) the ground-state, the model mass $M=(v/w)^2$, the magnetization, and the susceptibility of the 2D polaron are continuous functions of the electron-phonon constant α and the magnetic field ω_c. However, for $\alpha>1.60$ the polaron undergoes a transition from a "dressed state" $[M=(v/w)^2\gg 1]$ to a "stripped state" $[M=(v/w)^2\simeq 1]$. The transition is similar to that found for the 3D-polaron (see Ref. 6) case and for the problem of an electron on a liquid helium film.[13] We

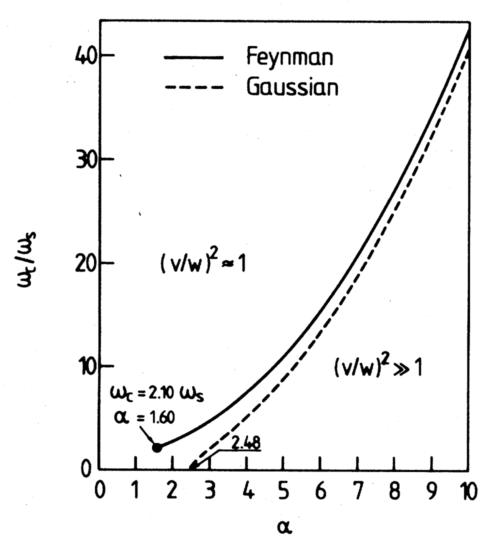

FIG. 6. Phase diagram for the polaron as obtained in the generalized Feynman approximation and in the Gaussian approximation.

refer to Refs. 6 and 13 for further details on the physics of this "polaron stripping transition."

The discontinuity in the polaron state is shown much more clearly in the behavior of the magnetization $\tilde{\mu}$ and the susceptibility $\tilde{\chi}$. At the point where the discontinuous transition starts to occur, i.e., $\alpha=1.60\pm0.01$, $\omega_c=2.10\pm0.01$ (see Fig. 1), $\tilde{\mu}$ is still continuous, but $\tilde{\chi}$ diverges which is reminiscent of a critical point where the transition is of second order. For $\alpha>1.60$, both $\tilde{\mu}$ and $\tilde{\chi}$ are discontinuous at a certain value of the magnetic field (see Figs. 1–4). The transition behavior of the polaron is summarized in Fig. 5 where the magnetic field at which the transition occurs is plotted versus the inverse of the electron-phonon coupling constant.

The effect of the electron-phonon interaction on the properties of the polaron are enhanced in two dimensions

TABLE I. Polaron ground-state energy for $\alpha=0.1$, 1.0, and 4 for different values of the magnetic field strength within the generalized Feynman approximation (E_{present}) and within the Gaussian approximation (E_{Gaussian}). The mass of the Feynman polaron model $M=(v/w)^2$ is also given.

ω_c/ω_s	E_{present}	E_{Gaussian}	$(v/w)^2$
		$\alpha=0.1$	
0.0	−0.157 54	−0.157 08	1.036
0.1	−0.109 51	−0.109 05	1.039
0.2	−0.061 49	−0.061 05	1.042
0.4	0.034 51	0.034 92	1.046
0.6	0.130 49	0.130 86	1.045
0.8	0.226 47	0.226 80	1.043
1.0	0.322 47	0.322 75	1.038
1.5	0.562 61	0.562 80	1.022
2.0	0.803 00	0.803 13	1.014
4.0	1.767 59	1.767 63	1.004
10.0	4.682 67	4.682 67	1.000
		$\alpha=1.0$	
0.0	−1.623 22	−1.570 80	1.530
0.1	−1.592 02	−1.540 55	1.565
0.2	−1.560 80	−1.510 49	1.604
0.4	−1.498 15	−1.450 81	1.674
0.6	−1.435 09	−1.391 40	1.737
0.8	−1.371 52	−1.332 01	1.783
1.0	−1.307 39	−1.272 45	1.795
1.5	−1.145 16	−1.122 04	1.511
2.0	−0.983 30	−0.968 70	1.221
4.0	−0.327 48	−0.323 74	1.039
10.0	1.826 27	1.826 71	1.005
		$\alpha=4.0$	
0.0	−8.2074	−7.6945	76.78
0.1	−8.2067	−7.6944	76.88
0.2	−8.2057	−7.6940	77.02
0.4	−8.2031	−7.6927	77.33
0.6	−8.1996	−7.6904	77.69
0.8	−8.1952	−7.6872	78.10
1.0	−8.1899	−7.6832	78.57
1.5	−8.1728	−7.6691	79.93
2.0	−8.1502	−7.6496	81.59
4.0	−8.0090	−7.5194	90.77
10.0	−7.7004	−6.7286	1.021

as compared to the 3D case (see Refs. 2—5). As a consequence the critical electron-phonon coupling constant and critical magnetic field strength, at which the transition starts to become discontinuous, are smaller in 2D than in the case of the 3D polaron,[6] where it was found that $\alpha=4.20$ and $\omega_c=2.24$. However, in terms of the behavior of the 2D polaron and the 3D polaron at the transition point, there are no qualitative differences.

For comparison, the ground-state energy, the magnetization (see Fig. 3), and the susceptibility (see Fig. 4) are also calculated for the Gaussian approximation which is obtained from Eq. (10) by putting $w=0$, in which case we are left with only one variational parameter. In Table I we compare the resulting values for the ground-state energy with the results from the generalized Feynman approximation presented here. It is obvious that our generalized Feynman approximation gives lower values for the ground-state energy than the Gaussian approximation. It is interesting to note that for $\alpha<2.48$ the ground-state energy obtained from the Gaussian approximation is, for all ω_c, identical to the result given by second-order Rayleigh-Schrödinger perturbation theory [this result is given by Eq. (12)]. The reason is that for $\alpha<2.48$ the variational parameter v in the Gaussian approximation is zero for *all* values of the magnetic field.

In Fig. 6 we compare the discontinuous behavior of both approximations with each other. Note that the Gaussian approximation gives, as a function of α, a first-order transition for all values of ω_c, even for $\omega_c=0$. As discussed in Ref. 8 (see also Ref. 9) this behavior is an *artifact of the Gaussian approximation.*

IV. CONCLUSION

We have recently found in Ref. 8 that the Feynman approximation to the polaron ground-state energy in 2D (E_{2D}) can be obtained from the 3D result (E_{3D}) by using the scaling relation $E_{2D}(\alpha)=\frac{2}{3}E_{3D}(3\pi\alpha/4)$. This scaling relation breaks down when a magnetic field is applied, the reason being that the scaling relation results from the fact that in the Feynman approximation for $\omega_c=0$ the components of the motion of the electron in the different space directions do not couple with each other and are treated within the same approximation. But a magnetic field introduces a special direction into the problem and destroys this spherical symmetry which as a consequence implies that E_{2D} can no longer be obtained from E_{3D} by the scaling relation of Ref. 8.

The "stripping transition" of the polaron found in the present paper is analogous to the one found for the 3D polaron by two of the authors in Ref. 8. Recently a similar transition was found for an electron on a liquid-helium film.[13] There the electrons interact with the surface excitations of the liquid-helium film which are called ripplons (this problems can be mapped into a 2D acoustic polaron problem). For such a system it was found in Ref. 13 that the effect of the transition is much more dramatic and could lead to a change in the model mass $M=(v/w)^2$ of 5—6 orders of magnitude.

The discontinuity of the polaron state found in 2D for $\alpha>1.60$ and which occurs at a well-defined magnetic field strength is obtained within a generalization of the Feynman approximation as presented in Ref. 6 for the 3D polaron. One may argue that this discontinuity can be an artifact of the present approximation and may not be a property of the Fröhlich Hamiltonian. Concerning this point one may reflect on the discussion on the absence of a discontinuous self-trapping transition of the Fröhlich polaron as was presented in Ref. 9 (see also Ref. 14). Note also that within a variation scheme it is impossible to prove the existence of a phase transition.

In conclusion, on physical grounds, it is intuitively clear that as a function of the magnetic field there should be two regions: (i) a relatively small magnetic field region in which the polaron as an effective particle moves as a rigid entity, and (ii) a high magnetic field region in which the electron oscillates so rapidly that the phonon cloud is no longer able to follow the electron. Whether or not the transition from the dressed polaron state to the stripped polaron state is continuous or discontinuous is open to discussion. We found that within the generalized Feynman approximation the transition is continuous for materials with $\alpha<1.60$ and discontinuous when $\alpha>1.60$.

The fact that confinement of the electron motion to two space dimensions enhances the polaron effects in comparison with polaron motion in 3D implies that the critical coupling in 2D, $\alpha=1.60$, is reduced in comparison with the critical coupling in 3D where $\alpha=4.20$. As a consequence a larger number of materials are available in which, from the present study, we expect that the polaron undergoes a stripping transition as a function of the magnetic field if the electron motion is confined to 2D. For example, the present calculation predicts that for a heterostructure of AgCl ($\alpha=1.84$) a discontinuity occurs for $\omega_c/\omega_{LO}\sim 2.6$ or at a magnetic field of about $B\sim 140$ T. In this calculation we neglected the finite width of the electron layer and temperature effects (which is expected to be valid at helium temperatures). The transition should be visible in a cyclotron resonance experiment in which we expect a sudden narrowing of the cyclotron resonance line due to the sudden decrease in the *effective* electron-phonon interaction. At the transition point, the polaron cyclotron resonance spectrum transforms to the spectrum of a quasifree electron in a magnetic field.

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