ON THE THEORY OF THE PIEZOELECTRIC POLARON

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The interaction of an electron with acoustic phonons in piezoelectric crystals is investigated. It is shown that because of the infrared divergence the electron Green's function does not have a pole at $\epsilon = p^2/2$, but has a branch point instead. As a consequence the electron density of states has the form $\rho(\epsilon) \sim \epsilon^{1\,2+2\alpha/\pi}$ for small values of ϵ, where α is the coupling constant.

1. INTRODUCTION

INTEREST in the polaron problem is due to the fact that the polaron represents a simple example of the interaction of a particle with a quantized field, and also because this problem is essential in order to understand the motion of electrons in ionic crystals. The problem of an electron interacting with acoustic phonons in piezoelectric crystals serves as another interesting example of the interaction of a particle with a field.

The Hamiltonian of the system has the form[1,2]

$$H=\frac{p^2}{2}+\sum_q\left(a_q^+a_q+\frac{1}{2}\right)q+\left(\frac{4\pi\alpha}{V}\right)^{1/2}\sum_q\frac{1}{\sqrt{q}}(a_q+a_{-q}^+)e^{iqr}. \quad (1)$$

Here the unit of energy is ms^2, and the unit of length is $\hbar/ms$; s is the speed of sound. The coupling constant α is given by

$$\alpha=\frac{\hbar/ms}{\hbar^2\varepsilon/me^2}\frac{\langle e_{ijk}^2\rangle}{2\varepsilon c}, \quad (2)$$

where $\langle e_{ijk}^2 \rangle$ is an "averaged" square[2] of the piezoelectric tensor, ϵ is the dielectric constant, and c is the elastic constant.

Only the case of zero temperature, T = 0, and small values of the coupling constant will be considered in this article.

The problem of the spectrum of the piezoelectric polaron at zero temperature was first investigated by Whitfield et al.[2] They calculated the correction to the mass and the shift of the band edge in second-order perturbation theory. However, the treatment carried out in[2] is incorrect. As will be shown below, certain Feynman diagrams contain asymptotically logarithms of $|\eta|$ as $\epsilon \to p^2/2$, where

$$\eta = \varepsilon - p^2/2,$$

and the effective parameter of perturbation theory becomes $\alpha \ln|\eta|$.

The perturbation-theory series contains both powers of α and powers of $\alpha \ln|\eta|$. We shall assume that $\alpha \ll 1$ and we shall assemble the series in powers of $\alpha \ln|\eta|$.

2. THE VERTEX PART

In what follows it is convenient to transfer the complete matrix element of the interaction in (1) to the phonon Green's function, so that

$$D_0(\omega, \mathbf{k}) = 8\pi\alpha/(\omega^2 - \mathbf{k}^2 + i\delta). \quad (3)$$

The first correction to the scalar vertex Γ is shown in Fig. 1:

$$\Gamma_1 = i\int\frac{d\omega}{2\pi}\frac{d^3k}{(2\pi)^3}D_0(\omega,\mathbf{k})G_0(\varepsilon_1-\omega,\mathbf{p}_1-\mathbf{k})G_0(\varepsilon_2-\omega,\mathbf{p}_2-\mathbf{k}). \quad (4)$$

One can easily verify that after evaluating the integral with respect to the phonon frequency ω, the remaining integration with respect to the phonon momentum $\mathbf{k}$ contains a region $\max(|\eta_1|, |\eta_2|) \ll k \ll 1$ which gives a logarithmic contribution. For $p \ll 1$ the contribution from this region is given by

$$\Gamma_1 \approx \frac{2\alpha}{\pi}\ln\frac{1}{\max(|\eta_1|,|\eta_2|)}. \quad (5)$$

Thus, the correction to the vertex increases without any limit as both of the electron end points approach the mass surface $\epsilon = p^2/2$, The situation is analogous to the well-known problem of the infrared catastrophe in quantum electrodynamics, which has been discussed by Abrikosov.[3]

The second-order diagrams are shown in Fig. 2. The first diagram vanishes upon replacing the bare electron Green's function by the complete Green's function. One can show that the last diagram, containing two intersecting phonon lines, gives a contribution proportional to $\alpha^2 \ln|\eta|$, that is, it contains a smaller power of the logarithm than the power of the constant α. This also holds true in more complicated diagrams containing intersections of dotted lines. Therefore, such diagrams will not be taken into consideration in the leading approximation. This implies that we do not approach too close to the mass surface.

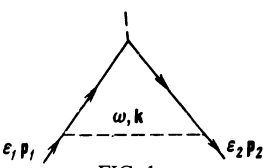

FIG. 1

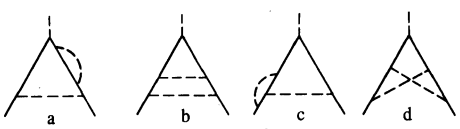

FIG. 2

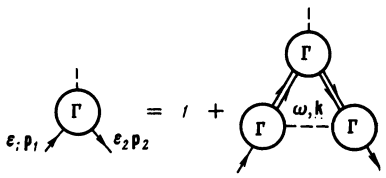

FIG. 3

Let us consider the corrections to the vector vertex $\vec{\Gamma} = \partial G^{-1}/\partial \mathbf{p}$. The bare vector vertex is given by $\vec{\Gamma}_0 = -\mathbf{p}$. From the structure of the perturbation-theory series it is clear that the equality

$$\vec{\Gamma} = -\mathbf{p}\Gamma. \tag{6}$$

is valid in the leading logarithmic approximation to all orders in α and for $p \ll 1$.

Thus, the summation of the leading logarithms reduces to the solution of the equation for the vertex Γ shown in Fig. 3. The double line represents the exact Green's function of the electron which can be expressed in terms of the scalar vertex Γ (to within logarithmic accuracy) by using the Ward's identities $\partial G^{-1}/\partial \epsilon = \Gamma$ and $\partial G^{-1}/\partial \mathbf{p} = \vec{\Gamma}$:

$$G(\varepsilon, \mathbf{p}) = G_0(\varepsilon, \mathbf{p})\Gamma^{-1}(\varepsilon, \mathbf{p}). \tag{7}$$

We note that the supplementary vertices in the second term on the right hand side of the equation shown in Fig. 3 cancel with the same factors in the exact expressions for the electron Green's functions, that is, the supplementary vertices Γ and G can remain bare.

Since Γ is by assumption a slowly varying function, the integration over the phonon frequency ω implies evaluating the residue at the pole of the phonon Green's function D_0. After this, in terms of logarithmic variables the equation shown in Fig. 3 takes the form

$$\Gamma(x) = 1 + \frac{2\alpha}{\pi}\int_0^x \Gamma(t)\,dt, \quad x = \ln(1/|\eta|), \quad t = \ln(1/k), \tag{8}$$

where $\eta \sim \eta_1 \sim \eta_2$. Solving this equation, we obtain $\Gamma = \exp\{2\alpha x/\pi\}$, that is

$$\Gamma(\varepsilon, \mathbf{p}) = |\eta|^{-2\alpha/\pi}. \tag{9}$$

3. THE DENSITY OF STATES

Let us compare the Green's function of the piezoelectric polaron,

$$G(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - p^2/2}\left(\frac{1}{\varepsilon - p^2/2}\right)^{-2\alpha/\pi} \tag{10}$$

with the Green's function in quantum electrodynamics[3]

$$G(p) = \frac{\hat{p} + m}{p^2 - m^2}\left(\frac{m^2}{p^2 - m^2}\right)^{\alpha_1(3-a_0)/2\pi}, \tag{11}$$

where $\alpha = 1/137$ and a_0 is the ratio of the coefficient associated with the longitudinal part of the phonon propagator to the coefficient associated with the transverse part. In the case of the transverse gauge (the Landau gauge) $a_0 = 0$, that is, the exponent in (11) is positive. In contrast to quantum electrodynamics, where there is an arbitrariness in the gauge of the photon propagator, in the present case the phonon Green's function is purely longitudinal. Therefore it is natural to compare formulas (10) and (11) for a gauge with $a_0 \gg 1$ (longitudinal photons). In fact, in this case the exponents in formulas (10) and (11) have identical signs.

If the density $\rho(\epsilon)$ of electronic states is calculated according to the formula

$$\rho(\varepsilon) = -\frac{2}{\pi}\int \frac{d^3p}{(2\pi)^3}\,\mathrm{Im}\,G(\varepsilon, \mathbf{p}) \tag{12}$$

then for $\epsilon \ll 1$ we obtain

$$\rho(\varepsilon) = \rho_0(\varepsilon)\varepsilon^{2\alpha/\pi}, \tag{13}$$

where $\rho_0(\epsilon) = \sqrt{2\epsilon}/\pi^2$ denotes the density of states in the absence of any interaction with the phonons.

In conclusion we note that the coupling constant α need not be very small in piezoelectric crystals; for example, $\alpha = 0.3$ in ZnO.[1] This circumstance permits us to hope for an experimental verification of the ideas presented above.

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