Slow Electrons in a Polar Crystal

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A variational principle is developed for the lowest energy of a system described by a path integral. It is applied to the problem of the interaction of an electron with a polarizable lattice, as idealized by Fröhlich. The motion of the electron, after the phonons of the lattice field are eliminated, is described as a path integral. The variational method applied to this gives an energy for all values of the coupling constant. It is at least as accurate as previously known results. The effective mass of the electron is also calculated, but the accuracy here is difficult to judge.

AN electron in an ionic crystal polarizes the lattice in its neighborhood. This interaction changes the energy of the electron. Furthermore, when the electron moves the polarization state must move with it. An electron moving with its accompanying distortion of the lattice has sometimes been called a polaron. It has an effective mass higher than that of the electron. We wish to compute the energy and effective mass of such an electron. A summary giving the present state of this problem has been given by Fröhlich.[1] He makes simplifying assumptions, such that the crystal lattice acts much like a dielectric medium, and that all the important phonon waves have the same frequency. We will not discuss the validity of these assumptions here, but will consider the problem described by Fröhlich as simply a mathematical problem. Aside from its intrinsic interest, the problem is a much simplified analog of those which occur in the conventional meson theory when perturbation theory is inadequate. The method we shall use to solve the polaron problem is new, but the pseudoscalar symmetric meson field problems involve so many further complications that it cannot be directly applied there without further development.

We shall show how the variational technique which is so successful in ordinary quantum mechanics can be extended to integrals over trajectories.

STATEMENT OF THE PROBLEM

With Fröhlich's assumptions, the problem is reduced to that of finding the properties of the following Hamiltonian:

$$H=\tfrac{1}{2}\mathbf{P}^2+\sum_K a_K^+a_K+i(\sqrt{2}\pi\alpha/V)^{\frac{1}{2}}\sum_K\frac{1}{K}\times[a_K^+\exp(-i\mathbf{K}\cdot\mathbf{X})-a_K\exp(i\mathbf{K}\cdot\mathbf{X})]. \quad (1)$$

Here $\mathbf{X}$ is the vector position of the electron, $\mathbf{P}$ its conjugate momentum, a_K^+, a_K the creation and annihilation operators of a phonon (of momentum $\mathbf{K}$). The frequency of a phonon is taken to be independent of $\mathbf{K}$. Our units are such that $\hbar$, this frequency, and the electron mass are unity. The quantity α acts as a coupling constant, which may be large or small. In conventional units it is given by

$$\alpha=\frac{1}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon}\right)\frac{e^2}{\hbar\omega}\left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}},$$

where ϵ, ϵ_∞ are the static and high frequency dielectric constant, respectively. In a typical case, such as NaCl, α may be about 5. The wave function of the system satisfies ($\hbar=1$)

$$i\partial\psi/\partial t=H\psi, \quad (2)$$

so that if φ_n and E_n are the eigenfunctions and eigenvalues of H,

$$H\varphi_n=E_n\varphi_n, \quad (3)$$

then any solution of (2) is of the form

$$\psi=\sum_n C_n\varphi_n e^{-iE_nt}.$$

Now we can cast (1) and (2) into the Lagrangian form of quantum mechanics and then eliminate the field oscillators (specializing to the case that all phonons are virtual). Doing this in exact analogy to quantum electrodynamics,[2] we find that we must study the sum over all trajectories $\mathbf{X}(t)$ of $\exp(iS')$, where

$$S'=\frac{1}{2}\int\left(\frac{d\mathbf{X}}{dt}\right)^2dt+2^{-\frac{1}{2}}\alpha i\int\int|\mathbf{X}_t-\mathbf{X}_s|^{-1}e^{-i|t-s|}dtds. \quad (4)$$

This sum will depend on the initial and final conditions and on the time interval T. Since it is a solution of the Schrödinger Eq. (2), considered as a function of T it will contain frequencies E_n, the lowest of which we seek. It is difficult to isolate the lowest frequency, however.

For that reason, consider the mathematical problem of solving

$$\partial\psi/\partial t=-H\psi, \quad (5)$$

without question as to the meaning of t. This has the same eigenvalues and eigenfunctions as (3), but a

[1] H. Fröhlich, Advances in Physics 3, 325 (1954). References to other work is given here.

[2] R. P. Feynman, Phys. Rev. 80, 440 (1950).