"Smoothing Out" of Charge Density in Polaron Theory

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IF the effective mass method (E.M.M.) is used in the polaron theory[1], one must solve an auxiliary equation for a "smoothed out" wave function

$$\left(-\frac{\hbar^2}{2\mu}\Delta + W\right)\varphi = E\varphi; \qquad \varphi = \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}, \quad (1)$$

where μ is the effective mass of an electron. The polarization potential $W(\mathbf{r})$ in Eq. (1) is not computed from the exact wave function (the so-called detailed wave function) of the polaron $\psi(\mathbf{r}) = \Sigma a_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r})$ ($\psi_{\mathbf{k}}$ is the Bloch wave function), i.e., not as $W_{|\psi|} = -e^2 c \int \frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} d\tau'$ but from a "smoothed out" function $\varphi(\mathbf{r})$. Such smoothing out of potential which brings Eq. (1) into a self-consistent form, introduces a definite error into the value of the computed energy. The purpose of the present letter is to evaluate the error committed when the criterion of applicability of E.M.M. $r_p \gg a$ (r_p is the polarization radius, a is the separation between neighboring ions) is barely met. Such is the case for the majority of the alkali-halide crystals.

Applying perturbation theory, we obtain for this error

$$E_1 = \int (W_{[\psi]} - W_{[\varphi]})\,|\varphi|^2 d\tau \quad (2)$$

$$= -e^2 c \int \frac{|\psi(\mathbf{r}')|^2\,|\varphi(\mathbf{r})|^2}{|\mathbf{r}-\mathbf{r}'|} d\tau\, d\tau'$$

$$+ e^2 c \int \frac{|\varphi(\mathbf{r})|^2\,|\varphi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} d\tau\, d\tau'.$$

We neglect here the dispersion of the crystal and the dependence of its polarization on the wave length, assuming $c = 1/n^2 - 1/\epsilon = \text{const}$. Because of considerations discussed by Tolpyg[2] we shall start from the approximation of strongly bounded electrons, according to which

$$\psi_k = \sum_{\mathbf{n}} e^{i\mathbf{k}\mathbf{n}} \psi_a(|\mathbf{r}-\mathbf{n}|),$$

where $\mathbf{n}$ is the radius vector to the center of a cell coinciding with the nucleus of the positively charged ion. Pekar[1] used a variation principle to replace the integration of Eq. (1) and, as an approximation, the following function may be used:

$$\varphi(r) = \frac{\alpha^{3/2}}{\sqrt{55\pi}}\left(1 + \alpha r + \frac{(\alpha r)^2}{2!} + \frac{(\alpha r)^3}{3!}\right) e^{-\alpha r},$$

where α is determined by minimizing the corresponding potential which yields

$$\alpha = 0.821\,(\mu/m)\,c/a_0,$$

where a_0 is the Bohr radius.

The second term of Eq. (2) is integrated directly after the substitution of $\varphi(\mathbf{r})$. The result is $0.2613\, e^2 c\,\alpha$ and, after substituting $\psi(\mathbf{r}) = \sum_{\mathbf{k}} a_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r})$, the first term of Eq. (2) has the form

$$\int W_{[\psi]}\,|\varphi|^2 d\tau = \Delta \sum_{\mathbf{n},\mathbf{n}'} \varphi(\mathbf{n})\,\varphi^*(\mathbf{n}') \quad (3)$$

$$\times \int \psi_a^*(|\mathbf{r}'-\mathbf{n}'|)\,\psi_a(|\mathbf{r}'-\mathbf{n}|)\; W_{[\varphi]}(\mathbf{r}')\, d\tau',$$

where Δ is the volume of the elementary cell.

We further demand (analogously to Tolpyg[2]) that $W(\mathbf{r})$ be expandable in a series of $(\mathbf{r}-\mathbf{n})$ within the boundaries of each cell. After substituting such expressions into Eq. (3) we obtain for the case $n = n'$

$$\sum_{\mathbf{n}} |\varphi(\mathbf{n})|^2 \left[\psi^0 W_{(n)} + \frac{\psi^{(2)}}{3!}\nabla^2 W_{(n)} + \frac{\psi^{(4)}}{5!}\nabla^4 W_{(n)} + \cdots\right],$$

$$\psi^{(2n)} = \int \psi_a(|\mathbf{r}-\mathbf{n}'|)\, r^{2n}\, d\tau.$$

The last expression is computed by passing from a sum over $\mathbf{n}$ to an integral. The terms with $n \neq n'$ in Eq. (3) are computed on the assumption that the maximum value of the integrand in the overlap integral lies midway between the lattice points, which follows from symmetry consideration. $W(\mathbf{r})$ is expanded in orders of $|\mathbf{r} - \tfrac{1}{2}(\mathbf{n}+\mathbf{n}')|$. The numerical calculation was carried out for the sodium salts. The function ψ_a was approximated

with sufficient accuracy from the data of Fock and Petrashen[3].

$$\psi_a(r) = 0.727\,(4\pi a_0^3)^{-1/2}\,(r/a_0 - 1)\,e^{-0.71r/a_B}.$$

The result is

$$E_1 = (0.01873\cdot 10^{-16}\alpha^2 + 0.07221\times 10^{-32}\,\alpha^4 + \cdots)\,e^2 c\alpha.$$

For example, for the crystal NaCl $\alpha = 1.109 \times 10^8$ and the error in Pekar's[1] energy evaluation due to smoothing out of the potential is about 15%, which lowers the computed energy value after Eq. (1) is brought to a self-consistent form. We note, however, that using the approximation of strongly bound electrons increases somewhat the estimate of the energy error, and in reality this error is only about 10-12% for NaCl.

Tolpyg[2] considered higher order terms in the E.M.M. and showed that the E.M.M. of Pekar overstates the energy values, for NaCl in particular by 12-13%. Thus, the above errors are approximately equal and in opposite directions, which verifies the applicability of E.M.M. for calculation of energies, even when r_p is greater than a by a factor of 2 or 3.

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[2] K. B. Tolpyg, J. Exptl. Theoret. Phys. (U.S.S.R.) 21, 443 (1951).

[3] V. A. Fock and M. Petrashen, Physik Z. d Sowjetunion 6, 369 (1934).

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On Annihilation of Antiprotons with Star Formation

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COLLISION of the antiproton with the proton and the annihilation of both particles results in the liberation of not less than 1.8×10^9 ev (if the velocities of both particles are small). This energy is sufficient for the formation of 13 π-mesons. It seems natural to apply to the investigation of stars of such high energy the statistical theory of multiple particle formation (see Refs. 1 and 2). The theory of thermodynamic variants leads to the following formula for the complete number of the formed particles[2,3].

$$N = k\,(E/Mc^2), \qquad (1)$$

where M denotes the mass of the nucleon and k is a coefficient determined from experiment. For large energies ($E \geq 10^{12}$ ev) $k \sim 2$. If this value of k is used with the energies of interest, $N \sim 2$. For such a small value of N the application of thermodynamics is not justified and we, therefore, turn to a variation of statistical theory suggested by Fermi[1] for the investigation of stars with the formation of not too many particles.

We shall start with the following formula (see Refs. 1, 4 and 5):

$$S(n) = f_{n,T}\,[\Omega/8\pi^3\hbar^3]^{n-1}\,W_n(E_0), \qquad (2)$$

The value of $S(n)$ determines the probability of meson formation, Ω the effective volume in which the energy of the colliding nucleons is concentrated and where the formation of particles takes place, E_0 the full energy of star formation, $W_n(E_0) = dQ_n(E_0)/dE_0$, $Q_n(E)$ the volume of the momentum space corresponding to the energy E_0, $f_{n,T}$ a factor accounting for the conservation of isotopic spin and the equivalence of particles (see Refs. 4 and 5), T the isotopic spin of the system. The effective volume was taken as $(4\pi/3)(\hbar/\mu c)^3$, where μ is the mass of the π^--meson. Justification for this selection was the fact that similar computations for multiple formation of particles for p-n and π^--p collisions result in a satisfactory agreement with experiment when the same expression is used for the evaluation of the effective volume[6]. It should be noted that the energy E_0 in these cases ~ 1 bev, i.e., not strongly different from the energy ~ 2 bev under consideration.

The magnitude of $W_n(E_0)$ has been computed in Ref. 7 with consideration for conservation of energy and momentum but on the assumption that the formed particles are ultrarelativistic. As it will be shown further this assumption is approxi-