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COMMENT

A note on the ground state of the bound polaron†

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Abstract. It is shown that the action in Feynman's representation of the Hamiltonian of the free polaron may be approximated by a Coulombic term in the strong coupling limit. This leads to an analytic approximation for the ground state energy of a bound polaron.

In a now well known paper Feynman (1955) showed that the ground state energy of a polaron could be calculated from a path integral of the following form (see also discussions by Schultz 1963 and Feynman and Hibbs 1965):

$$K(\boldsymbol{r}, t, \boldsymbol{r}', t') = \int \mathscr{D}[\boldsymbol{r}(\tau)] \exp\left[-\frac{1}{2}\int \left(\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\tau}\right)^2 + \frac{\alpha}{2^{3/2}}\iint \mathrm{d}\tau\,\mathrm{d}\sigma\,\frac{\mathrm{e}^{-|\tau-\sigma|}}{|\boldsymbol{r}(\tau)-\boldsymbol{r}(\sigma)|}\right]. \tag{1}$$

The ground state energy was shown by Feynman to be obtainable from a variational principle. Choosing a trial action so as to approximate the action S in (1), Feynman showed that if E_0, E are the corresponding ground state energies,

$$E \leqslant E_0 - S \tag{2}$$

where

$$\lim_{t'-t\to\infty} \langle S - S_0 \rangle = s(t'-t) \tag{3}$$

and for any functional $F[\boldsymbol{r}(\tau)]$

$$\langle F \rangle = \frac{\int \mathrm{e}^{S_0} F \mathscr{D} r(\tau)}{\mathrm{e}^{S_0} \mathscr{D} r(\tau)}. \tag{4}$$

In his original paper Feynman mentions trying various actions, such as the free particle and Coulombic, before finding a brilliantly successful trial action valid for all ranges of the coupling constant.

In this note we are concerned with the bound polaron, ie the polaron in the Coulombic field. It can be shown (Schultz 1963) that the action for this case can be written in the form

$$S = -\frac{1}{2}\int_0^T \left(\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\tau}\right)^2 \mathrm{d}\tau - \int_0^T \frac{\beta}{|\boldsymbol{r}(\tau)|}\,\mathrm{d}\tau + \frac{\alpha}{2^{3/2}}\int_0^T\int_0^T \frac{\mathrm{e}^{-|\tau-\sigma|}}{|\boldsymbol{r}(\tau)-\boldsymbol{r}(\sigma)|}\,\mathrm{d}\tau\,\mathrm{d}\sigma \tag{5}$$

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where

$$\alpha = \frac{\beta}{\sqrt{2}}\left(\frac{\epsilon}{\epsilon_\infty} - 1\right)$$

in the units chosen. Calculations have been carried out by Platzman (1962) for this case and other methods are reviewed by Bajaj (1972). Essentially we are concerned here with the point that for the bound polaron problem there is an obvious advantage in representing S_0 by a Coulombic action, and we succeed in obtaining an analytic approximation for the ground state energy valid for the strong coupling case.

Consider the problem of evaluating equation (3) for an arbitrary trial action S_0. If $K_0(\boldsymbol{r}_1, \boldsymbol{r}', \beta)$ denotes the corresponding propagator, the average over S is given by

$$\langle S\rangle = \iint K_0(0, \boldsymbol{r}, \beta, \tau)\frac{e^{-|\tau_1-\tau_2|}}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}K_0(\boldsymbol{r}_1, \boldsymbol{r}_2, \tau_1, \tau_2)K_0(\boldsymbol{r}_2, 0, \tau_2, 0)\,d\tau_1\,d\tau_2\,d\boldsymbol{r}_1\,d\boldsymbol{r}_2. \tag{6}$$

For the bound polaron there is an obvious advantage in attempting to represent S_0 by a Coulombic term which will add to the external Coulomb field. This suggests taking $S_0 = -Ze^2/r$ with Z a variational parameter. To carry such a programme through involves, however, knowledge of the function $K_0(\boldsymbol{r}, \boldsymbol{r}', t, t')$ for a Coulombic potential. Although some knowledge of this function exists (eg Schwinger 1964), none of the results available appears to be simpler than the eigenfunction expansion

$$K_0(\boldsymbol{r}, \boldsymbol{r}', t, t') = \sum_n \psi_n(\boldsymbol{r})\psi_n(\boldsymbol{r}')\,e^{-E_n(t-t')} \tag{7}$$

where the $\psi_n(\boldsymbol{r})$ are the eigenstates of the Coulomb potential. Two extreme approximations can be made. For the continuum part of the spectrum we can approximate the $\psi_n(\boldsymbol{r})$ by free particle wavefunctions, which is equivalent to approximation of K_0 by the free particle propagator. This result gives after considerable algebra

$$E = -\alpha \tag{8}$$

which is already known to be correct for weak coupling. The second, perhaps obvious approximation, is to argue that if the ground state is well separated from other states and from the continuum, then

$$K_0(\boldsymbol{r}, \boldsymbol{r}', t, t') \simeq \psi_0(\boldsymbol{r})\psi_0(\boldsymbol{r}')\,e^{-E_0(t-t')} \tag{9}$$

where $\psi_0(\boldsymbol{r})$ is the ground state wavefunction for the Coulomb potential. Some calculation now gives

$$\langle S - S_0\rangle = \frac{4\alpha\pi 2^{-3/2}}{8Z^2} - \frac{\pi}{2}. \tag{10}$$

The value of E can now be minimized with respect to z. We obtain

$$Z = 5\alpha/2^{7/2}. \tag{11}$$

This leads to the ground state energy $E = -\frac{25}{256}\alpha^2$ which is a reasonable result for strong coupling. Our main point now is that (11) can be substituted back into (5) to give a total Coulombic potential

$$V(r) = -\frac{\beta}{r} - \frac{5\alpha}{2^{7/2}r} \tag{12}$$

so that the ground state energy of the bound polaron in this approximation is simply

$$E = -\frac{1}{2}\left(\beta + \frac{5\alpha}{2^{7/2}}\right)^2. \tag{13}$$

This result agrees closely with the one given by Platzman in the strong potential limit, $\beta \to \infty$:

$$E = -\frac{4\beta^2}{3\pi} - \frac{4\alpha\beta}{3\pi} - \frac{3\ln 2}{2\beta} - \frac{\alpha^2}{3\pi}.$$

The simple character of these results suggests that it may well be worthwhile to investigate the possibility of obtaining a better approximation to the Coulomb propagator so that an equivalent Coulomb potential valid for all values of the coupling constant is obtained.

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