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APPLICATION OF TWO-POINT PADÉ APPROXIMANTS TO SOME SOLID STATE PROBLEMS

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A simple application of the two-point Padé approximants to the problem of polaron [5] is presented in the following. A conduction electron in a polar crystal will polarize and distort the ion lattice in its neighborhood. The lattice polarization, in turn, acts back on the electron and lowers its energy. The system of electron and its accompanying self-consistent polarization field is called a polaron. The Hamiltonian for the polaron is [3]

$$(1)\qquad H = \sum_k \frac{\hbar^2 k^2}{2m} c_k{}^+ c_k + \hbar\Omega \sum_q (a_q{}^+ a_q + \tfrac{1}{2}) + H_1,$$

$$(2)\qquad H_1 = i\hbar\Omega \left(\frac{4\pi\alpha}{V}\right)^{1/2} \left(\frac{\hbar}{2m\Omega}\right)^{1/4} \sum_{k,q} \frac{1}{|q|}(a_q{}^+ - a_{-q}) c^+_{k-q} c_k.$$

Here Ω is the optical phonon frequency, $\hbar$ is the Planck's constant, $\alpha = e^2/2(1/\epsilon_\infty - 1/\epsilon_0)\ (2m/\Omega\hbar^3)^{1/2}$ is the dimensionless polaron coupling constant, e is the charge of the electron, m is the conduction-based mass, ϵ_0 and ϵ_∞ are the static and optical dielectric constants of the solid respectively, $a_q(a_q{}^+)$ is an operator which destroys (creates) a longitudinal optical phonon of wavevector q, and $c_k(c_k{}^+)$ is an operator which destroys (creates) an electron of momentum k. There are two limits in which an approximate solution of the Schrödinger equation for the Hamiltonian (1) can be obtained: the weak-coupling limit ($\alpha \ll 1$) and the strong-coupling limit ($\alpha \gg 1$). The weak-coupling expansions of the ground state energy and effective mass of the polaron are [5]:

$$(3)\qquad E_0/\hbar\Omega = -\alpha - 0.015\,92\alpha^2 - 0.00\,8765\alpha^3 + \cdots,$$

and

$$(4)\qquad m/m^* = 1 - \frac{\alpha}{6} + 0.02263\alpha^2 + \cdots,$$

where E_0 is the ground state energy and M* is the effective mass of the polaron. In the strong coupling limit, we have the following expansions due to [1] and [2] respectively:

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