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:

(5) $E_0/\hbar\Omega = -0.1088\alpha^2 - 2.83,$

and

(6) $m^*/m = 0.02\alpha^4 - 1.01\alpha^2.$

In order to obtain the value of E_0 and m^* for intermediate values of α, we construct two-point Padé approximants to these weak and strong coupling expansions as follows. Instead of determining all the coefficients $(a_0 \cdots a_N, b_1 \cdots b_M)$ of a Padé approximant

(7) $P([M, N]; Z) = \dfrac{a_0 + a_1Z + a_2Z^2 + \cdots + a_NZ^N}{1 + b_1Z + \cdots + b_MZ^M},$

from the expansion around $Z = 0$, now only half of the equations determining the coefficients will come from the expansion around $Z = 0$. The remaining equations are determined by the expansion around $Z = \infty$. The results of such a fit are displayed in [5]. The energy vs. momentum relation for the polaron has also been similarly determined. In order to determine the accuracy of such fits, we construct the two-point Padé approximants of same order to fit Feynman's variational results at the weak and the strong coupling limits. The result indicates that the error for $E_0(\alpha)$ is at most 6–7% and the error for $\ell n m^*$ is at most 21%.

The method of two-point Padé approximants has also been used to determine the melting density of an electron lattice [4]. Due to the presence of logarithmic terms in the high density expansion of the ground state energy, the two-point Padé approximants are constructed to fit $r_s^4(\partial^2 E_0/\partial r_s^2)$, where $r_s = (4\pi/3 \cdot \text{density})^{-1/3} \cdot (\text{Bohr radius})^{-1}$. When the Padé approximants are twice integrated, the resultant $E_0(r_s)$ has a van der Waals loop at $r_s \cong 14.3$ provided that the low density expansion of E_0 has a term of the form $-4/35\ tr_s^{-5/2}$, where $-2 \le t \le 7$ is a constant.

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