Reply to “On the cutoff parameter in the translation-invariant theory of the strong coupling polaron”

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Abstract

The present work is a reply to the paper \cite{1}. It is proven that the argumentation of Ref. \cite{1} is inconsistent. The variational functional for the polaron ground state energy considered in Ref. \cite{1} contains an incomplete recoil energy. Since the variational functional of Ref. \cite{1} is incomplete, it is not proven to provide a variational upper bound for the polaron ground-state energy. The same conclusion follows also for the bipolaron ground-state energy.

Keywords:
Polarons, Fröhlich Hamiltonian, Bipolarons

Polarons and bipolarons are invoked in the study of polar materials, including high-$T_c$ superconductors \cite{2, 3, 4}. Rigorous variational methods (see, e. g., Refs. \cite{5, 6, 7}) are important in this field, i. a. because in the bipolaron mechanism of superconductivity, the parameters of the superconducting state and the critical temperature strongly depend on the bipolaron binding energy. The work \cite{1} is a reply to our comments \cite{8} on the variational approach aimed at in Refs. \cite{9, 10, 11}. In Ref. \cite{8} we show that the strong-coupling expression for the bipolaron ground state energy calculated in Refs. \cite{9, 10} is not justified as a variational upper bound.

It is suggested in Ref. \cite{1} that a properly chosen cutoff for the phonon momenta leads to correct variational polaron and bipolaron ground-state energies in the strong-coupling limit. However, this conclusion is not valid, because the recoil energy treated in Refs. \cite{9, 10, 11} is incomplete, as we wrote in Ref. \cite{8}.

The complete polaron recoil energy within the approach of Ref. \cite{11} was found by Porsch and Rösseler \cite{12}. They showed that, when imposing a cutoff for the phonon momentum, the polaron recoil energy $E_R$ consists of two parts:

$$E_R = E_R^{(T)} + \delta E_R^{(PR)},$$

where $E_R^{(T)}$ is the recoil energy determined in Ref. \cite{11}, and the term $\delta E_R^{(PR)}$ is given by Eq. (43) of Ref. \cite{12}:

$$\delta E_R^{(PR)} = \frac{3\hbar}{2} \left( \Omega_{q_0} - \omega_{q_0} \right).$$

where $q_0$ is the cutoff value for the phonon momentum, $\omega_q = \omega_0 + \frac{q^2}{2m}$ with $\omega_0$ the LO-phonon frequency, and $\{\Omega_q\}$ are the frequency eigenvalues resulting from the Bogoliubov-like canonical transformation for the phonon operators (performed in Refs. \cite{11, 12}).

It is stated in the reply \cite{1} that the reasoning of Ref. \cite{8} is “based on the erroneous approach … to the strong coupling limit when the cutoff parameter is introduced in the theory.” However, the argumentation of Ref. \cite{1} is related only to the term $E_R^{(T)}$, ignoring the Porsch — Rösseler term $\delta E_R^{(PR)}$. In the present work we treat the contribution to the recoil energy $\delta E_R^{(PR)}$, missed in Refs. \cite{1, 2, 9, 10, 11}.

The expression obtained in Ref. \cite{12} for $\Omega_{q_0}$ reads

$$\Omega_{q_0} = \left\{ \omega_q^2 + \frac{1}{3} \int_0^1 d\eta \int_0^{q_0} dq \, \frac{\hbar^2 q^4}{3\pi^2 m} \left( \frac{1}{\omega_q + i\eta} + \frac{1}{\omega_q - i\eta} \right) \omega_q \right\}^{1/2} \times \left[ 1 + F(\omega_q + i\eta)^2 \right], \quad (3)$$

with the function

$$F(z) = \frac{\hbar}{6\pi^2 im} \int_0^{q_0} dq \, q^4 f^2 (q) \left( \frac{1}{\omega_q + z} + \frac{1}{\omega_q - z} \right). \quad (4)$$

Here, $f(q)$ are variational functions. In Ref. \cite{11}, they are chosen as

$$f(q) = -\frac{V_q}{\hbar \omega_0} \exp \left( -\frac{q^2}{2a^2} \right), \quad (5)$$

with the variational parameter $a$ and the amplitudes of the electron-phonon interaction $V_q$.

In Fig. 1, we plot the complete recoil energy $E_R$ and the contributions $E_R^{(T)}, \delta E_R^{(PR)}$ as a function of $a$ for $q_0 = 8$ and

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$a = 4$ (measured in units of $\sqrt{\frac{m\omega}{\hbar}}$). The arrow indicates the value of the coupling constant

$$\alpha_c = \sqrt{\frac{4a^4}{a^4}},$$

at which the steep maximum of the integrand in $E_R^{(T)}$ (mentioned in Ref. [11]) crosses the cutoff boundary.

For sufficiently small $\alpha$, the Tulub's recoil energy $E_R^{(T)}$ dominates, and $\delta E_R^{(PR)}$ is negligibly small. When $\alpha$ increases (keeping other parameters constant), $E_R^{(T)}$ tends to a finite value, while $\delta E_R^{(PR)}$ monotonically increases.

![Figure 1: The recoil energy $E_R$ (solid black curve), the contributions $E_R^{(T)}$ (dashed red curve) and $\delta E_R^{(PR)}$ (dotted green curve) as a function of $\alpha$ for $q_0 = 8$ and $a = 4$. The dot-dashed blue curve is the recoil energy without cutoff.]()