Second-Order Correction to Feynman's Path-Integral Calculation of the Polaron Self-Energy

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The second-order term of a series expansion for the exact Feynman path-integral expression for the polaron self-energy is calculated. For all values of the polaron coupling constant, the result yields a correction of less than 2% to Feynman's variational approximation of the polaron self-energy.

In a description of the motion of a single conduction electron in an ionic semiconductive crystal, Fröhlich[1] has developed a Hamiltonian for the system consisting of the electron interacting with the macroscopic polarization field resulting from the long-wavelength longitudinal-optical modes of the crystal. Fröhlich's Hamiltonian is given by

$$H(\alpha) = -\frac{1}{2}\frac{\partial^2}{\partial \vec{x}^2} + \sum_{\vec{v}} b_{\vec{v}}^{\dagger} b_{\vec{v}} + i\left(\frac{\sqrt{2}\,\pi\alpha}{S}\right)^{1/2} \times \sum_{\vec{v}} |\vec{v}|^{-1}(b_{\vec{v}}^{\dagger} e^{-i\vec{v}\cdot\vec{x}} - b_{\vec{v}} e^{i\vec{v}\cdot\vec{x}}) \quad , \tag{1}$$

where $\vec{x}$ is the electron coordinate, $b_{\vec{v}}^{\dagger}$ and $b_{\vec{v}}$ are bosonic creation and destruction operators of a polarization field quantum of wave vector $\vec{v}$, α is a dimensionless coupling constant characteristic of the crystal, and S is the normalization volume. The limit $S \to \infty$ is to be taken with

$$\lim \textstyle\sum_{\vec{v}} = S(2\pi)^{-3} \int d^3v \quad \text{as } S \to \infty \quad . \tag{2}$$

A natural unit system is employed in which $\hbar = \omega = m = 1$, where ω is the frequency of the long-wavelength longitudinal-optical modes and m is the Bloch mass of the electron.

The name "polaron" has been given to the entity consisting of the Bloch conduction electron together with its accompanying nonradiative polarization field. Accordingly, Fröhlich defines the polaron self-energy $E_0(\alpha)$ as the least eigenvalue of $H(\alpha)$. Feynman[2] has obtained an exact expression for the self-energy in terms of a Feynman path integral, namely,

$$E_0(\alpha) = -\lim_{T\to\infty}[T^{-1}\ln(\textstyle\int_{\vec{0},0}^{\vec{0},T} e^{-S} D\vec{x}(t))] \quad , \tag{3}$$

where

$$S = \int_0^T \frac{1}{2}\left(\frac{d\vec{x}(\tau)}{d\tau}\right)^2 d\tau - \alpha 8^{-1/2}\int_0^T\int_0^T e^{-|\tau-\sigma|}\,|\vec{x}(\tau) - \vec{x}(\sigma)|^{-1}\, d\tau\, d\sigma \quad . \tag{4}$$

The integral in Eq. (3) is a Feynman path integral over paths $\vec{x}(t)$ satisfying the boundary conditions $\vec{x}(0) = \vec{x}(T) = \vec{0}$.

Feynman[2] has employed a variational principle for obtaining an overestimate to the self-energy. Feynman's result E_F can be expressed as the sum of the zeroth- and first-order terms of the series expansion of Eq. (3) in powers of

$$\Delta S \equiv S - S' \quad , \tag{5}$$

where S' purports to approximate S and is given by

$$S' = \int_0^T \frac{1}{2}\left(\frac{d\vec{x}(\tau)}{d\tau}\right)^2 d\tau + \frac{1}{2}C\int_0^T\int_0^T e^{-w|\tau-\sigma|}[\vec{x}(\tau) - \vec{x}(\sigma)]^2\, d\tau\, d\sigma \quad , \tag{6}$$

wherein C and w are variational parameters chosen to minimize E_F. The superiority of Feynman's variational result to other approximations for the polaron self-energy as well as for the self-energy of an exactly solvable one-dimensional analog[3] of the polaron problem suggests that the series expansion of Eq. (3) may be rapidly convergent. Accordingly, it is the purpose of this paper to evaluate the second-order term in the expansion. Since the series carried to second order is not variational, the values of the parameters C and w which minimize Feynman's variational result E_F are still to be employed.

The expansion of Eq. (3) as a power series in ΔS can be written as

$$E_0(\alpha) = E_F + \Delta E_2 + O((\Delta S)^3) \quad , \tag{7}$$

where E_F is Feynman's variational answer given by

$$E_F = -\lim_{T\to\infty}\{T^{-1}\ln[\textstyle\int_{\vec{0},0}^{\vec{0},T} e^{-S'} D\vec{x}(t)] - T^{-1}\langle\Delta S\rangle\} \tag{8}$$

and where ΔE_2 is the second-order term given by

$$\Delta E_2 = -\lim_{T\to\infty}[(2T)^{-1}\langle(\Delta S - \langle\Delta S\rangle)^2\rangle] \quad . \tag{9}$$

The angular brackets in Eqs. (8) and (9) denote a path average defined by

$$\langle f[\vec{x}(t)]\rangle \equiv \int_{\vec{0},0}^{\vec{0},T} f[\vec{x}(t)] e^{-S'} D\vec{x}(t) \Big/ \int_{\vec{0},0}^{\vec{0},T} e^{-S'} D\vec{x}(t) \quad . \tag{10}$$

For the purpose of reduction, Feynman's self-energy, given by Eq. (8), and the second-order correction term, given by Eq. (9), may be written as

$$E_F = 3(v-w)^2(4v)^{-1} - \lim_{T\to\infty} A \tag{11}$$

and

$$\Delta E_2 = -\frac{1}{2}\lim_{T\to\infty}\left[\frac{\langle V^2[\vec{x}(t)]\rangle - T^2A^2}{T} - C\left(\frac{\partial}{\partial C}\Big|_{T,\alpha,w}(2A+B)\right)+B\right] \quad , \tag{12}$$

where

$$V[\vec{x}(t)] = -\alpha 8^{-1/2}\int_0^T\int_0^T e^{-|\tau-\sigma|}\,|\vec{x}(\tau)-\vec{x}(\sigma)|^{-1}\,d\tau\,d\sigma \quad , \tag{13}$$

$$A = -\langle V[\vec{x}(t)]\rangle/T \quad , \tag{14}$$

$$B = \tfrac{1}{2}CT^{-1}\int_0^T\int_0^T e^{-w|\tau-\sigma|}\langle[\vec{x}(\tau)-\vec{x}(\sigma)]^2\rangle\,d\tau\,d\sigma \quad , \tag{15}$$

and

$$v \equiv [w^2+(4C/w)]^{1/2} \quad . \tag{16}$$

In order to evaluate $\langle V^2[\vec{x}(t)]\rangle$, A, and B, it is convenient to introduce the generating function

$$W[\vec{f}(t)] \equiv \langle \exp[\int_0^T \vec{f}(t)\cdot\vec{x}(t)dt]\rangle \quad . \tag{17}$$

Then

$$A = \alpha 8^{-1/2}T^{-1}\int_0^T\int_0^T\int e^{-|\tau-\sigma|}(2\pi^2k^2)^{-1}W[\vec{f}_{\vec{k}}(t)]\,d^3k\,d\tau\,d\sigma \quad , \tag{18}$$

$$B = \tfrac{1}{2}CT^{-1}\int_0^T\int_0^T e^{-w|\tau-\sigma|}\{-\nabla_{\vec{k}}^2 W[\vec{f}_{\vec{k}}(t)]\}_{\vec{k}=\vec{0}}\,d\tau\,d\sigma \quad , \tag{19}$$

and

$$\langle V^2[\vec{x}(t)]\rangle = \alpha^2 8^{-1}T^2\int_0^T\int_0^T\int_0^T\int_0^T\int\int e^{-|\tau-\sigma|}e^{-|\tau'-\sigma'|} \times(2\pi^2k^2)^{-1}(2\pi^2k'^2)^{-1}W[\vec{f}_{\vec{k},\vec{k}'}(t)] \times d^3k\,d^3k'^3\,d\tau\,d\sigma\,d\tau'\,d\sigma' \quad , \tag{20}$$

where

$$\vec{f}_{\vec{k}}(t) = i\vec{k}[\delta(t-\tau)-\delta(t-\sigma)] \tag{21}$$

and

$$\vec{f}_{\vec{k},\vec{k}'}(t) = i\vec{k}[\delta(t-\tau)-\delta(t-\sigma)] + i\vec{k}'[\delta(t-\tau')-\delta(t-\sigma')] \quad . \tag{22}$$

The generating function defined by Eq. (17) may be evaluated by the method outlined in Ref. 2. The result is

$$W[\vec{f}(t)] = \exp\left[-\int_0^T \frac{1}{2}\left(\frac{d\vec{x}'(t)}{d(t)}\right)^2 dt - \frac{1}{2}C\int_0^T\int_0^T e^{-w|t-\sigma|}[\vec{x}'(t)-\vec{x}'(\sigma)]^2\,dt\,d\sigma + \int_0^T \vec{f}(t)\cdot\vec{x}'(t)\,dt\right] \quad , \tag{23}$$

where each rectangular component $x_i'(t)$ of $\vec{x}'(t)$ is the solution to the equation

$$\frac{d^2x_i'(t)}{dt^2} = 2C\int_0^T e^{-w|t-\sigma|}[x_i'(t)-x_i'(\sigma)]\,d\sigma - f_i(t) \quad , \tag{24}$$

subject to boundary conditions $x_i'(0) = x_i'(T) = 0$, where $f_i(t)$ is the ith rectangular component of $\vec{f}(t)$. Apart from transient terms which are appreciable only near $t=0$ and $t=T$ and which will be irrelevant in the required limit $T\to\infty$,

$$\vec{x}'(t) = -(2v^2)^{-1}\int_0^T F(|t-t'|)\vec{f}(t')\,dt' + \text{const} \tag{25}$$

where, in the limit $T\to\infty$,

$$F(t) = (v^2-w^2)v^{-1}(1-e^{-vt}) + w^2t \quad . \tag{26}$$

In obtaining this result, use has been made of the property of $\vec{f}_{\vec{k}}(t)$ and $\vec{f}_{\vec{k},\vec{k}'}(t)$ that

$$\int_0^T \vec{f}(t)\,dt = \vec{0} \quad . \tag{27}$$

Substitution of Eqs. (23) and (25) into Eqs. (18)–(20) yields, upon reduction,

$$E_F = 3(v-w)^2(4v)^{-1} - 2\alpha v\pi^{-1/2} \times\int_0^\infty \rho\exp(-\rho^2)F^{-1/2}(\rho^2)\,d\rho \tag{28}$$

and

$$\Delta E_2 = -4\alpha^2v^2\pi^{-1}I + \alpha v^{-1}(v^2-w^2)\pi^{-1/2}\int_0^\infty \rho\exp(-\rho^2) \times F^{-1/2}(\rho^2)\,d\rho - \tfrac{3}{16}(v^2-w^2)^2v^{-3} - \tfrac{1}{2}\alpha(v^2-w^2)\pi^{-1/2}$$

TABLE I. Numerical results for variational parameters and self-energy values.

α	v	w	E_F	ΔE_2	E_c	% correction to E_F
1	3.110	2.871	−1.01	−0.0035	−1.02	0.35
3	3.421	2.560	−3.13	−0.031	−3.16	1.0
5	4.034	2.140	−5.44	−0.083	−5.52	1.5
7	5.810	1.604	−8.11	−0.13	−8.24	1.6
9	9.850	1.282	−11.5	−0.17	−11.7	1.4
11	15.41	1.162	−15.7	−0.22	−15.9	1.4
15	30.08	1.076	−26.7	−0.39	−27.1	1.5

$$\times \int_0^\infty \rho \exp(-\rho^2) F^{-3/2}(\rho^2)\{(1+w^2v^{-2})[1-\exp(-v\rho^2)] + (v^2-w^2)v^{-1}\rho^2\exp(-v\rho^2)\}d\rho \ , \tag{29}$$

where

$$I = \int_0^\infty\int_0^\infty\int_0^\infty [\rho_1\exp(-\rho_1^2)F^{-1/2}(\rho_1^2)] \times [\rho_2\exp(-\rho_2^2)F^{-1/2}(\rho_2^2)] \times [Q^{-1}\arcsin(Q)-1]d\rho_1\,d\rho_2\,d\rho_3 \ , \tag{30}$$

with

$$\begin{aligned} &Q=Q_1 \quad \text{for} \quad \rho_3-\rho_2^2+\rho_1^2\geq 0 \quad \text{and} \quad \rho_3-\rho_2^2\geq 0, \\ &Q=Q_2 \quad \text{for} \quad \rho_3-\rho_2^2+\rho_1^2\geq 0 \quad \text{and} \quad \rho_3-\rho_2^2< 0, \\ &Q=Q_3 \quad \text{for} \quad \rho_3-\rho_2^2+\rho_1^2< 0 \quad \text{and} \quad \rho_3-\rho_2^2< 0, \end{aligned} \tag{31}$$

wherein

$$Q_1 = \tfrac{1}{2}F^{-1/2}(\rho_1^2)F^{-1/2}(\rho_2^2)(v^2-w^2)v^{-1}e^{-v\rho_3} \times (1-e^{-v\rho_1^2})(e^{v\rho_2^2}-1) \ , \tag{32}$$

$$Q_2 = \tfrac{1}{2}F^{-1/2}(\rho_1^2)F^{-1/2}(\rho_2^2)\{(v^2-w^2)v^{-1}[e^{-v(\rho_2^2-\rho_3)} - e^{-v\rho_3}(1+e^{-v(\rho_1^2-\rho_2^2)}-e^{-v\rho_1^2})]-2w^2(\rho_2^2-\rho_3)\}, \tag{33}$$

and

$$Q_3 = -\tfrac{1}{2}F^{-1/2}(\rho_1^2)F^{-1/2}(\rho_2^2)\{(v^2-w^2)v^{-1}[e^{-v\rho_3} \times (1-e^{-v\rho_1^2})+e^{-v(\rho_2^2-\rho_3)}(e^{v\rho_1^2}-1)]+2w^2\rho_1^2\}. \tag{34}$$

Although the integrals in Eqs. (28)–(30) must be evaluated numerically, weak and strong coupling expansions may be obtained from them by following the approach described in Ref. 2. For weak coupling

$$E_F = -\alpha-(1/81)\alpha^2+O(\alpha^3) \approx -\alpha-0.01235\alpha^2+O(\alpha^3) \ , \tag{35}$$

and the corrected energy E_c is given by

$$E_c \equiv E_F+\Delta E_2 = -\alpha-a_c\alpha^2+O(\alpha^3) \approx -\alpha-0.01592\alpha^2+O(\alpha^3) \ , \tag{36}$$

where

$$a_c = \ln(1+3\sqrt{2}/4)-1/\sqrt{2} \ . \tag{37}$$

This corrected energy expression E_c is identical with the result of the fourth-order perturbation expansion for the self-energy, which is exact to second order in α. For strong coupling

$$E_F = -(3\pi)^{-1}\alpha^2+O(\alpha^0) \approx -0.1061\alpha^2+O(\alpha^0) \tag{38}$$

and the corrected energy is

$$E_c = -b_c\alpha^2+O(\alpha^0) \approx -0.1078\alpha^2+O(\alpha^0) \ , \tag{39}$$

where

$$b_c = (4\pi)^{-1}+2\pi^{-1}\sum_{n=1}^{\infty}\frac{(2n)!}{2^{4n}(n!)^2n(2n+1)} \ . \tag{40}$$

This refinement amounts to only a 1.6% correction to Feynman's strong coupling result for the self-energy.

For intermediate values of α, computer programs were written to calculate the integrals in Feynman's variational expression, given by Eq. (28), and in the second-order correction term, given by Eqs. (29)–(34). The values obtained for the variational parameters v and w by numerically minimizing Feynman's variational expression E_F disagree slightly with those reported by Schultz[4] and are given in Table I accurately apart from an uncertainty of ±1 in the fourth significant digit. For these values of v and w, Feynman's self-energy, its second-order correction, the corrected value, and the percentage correction were calculated and are all given in Table I accurately to within an uncertainty of at most ±1 in the least significant digit reported.

In conclusion, the second-order correction term represents less than a 2% correction to Feynman's variational answer for all values of α. This conclusion is suggestive that further corrections to the self-energy would be rather insignificant.

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Brillouin-Zone–Fermi-Surface Interactions in Pure and Lead-Doped Indium†

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Electrical resistivity anisotropies ($a \equiv \rho_\perp/\rho_\parallel$, direction referred to the c axis) of pure indium containing 0–9-at.% lead have been measured at 4.2, 77, and 273 °K. For pure indium it was found that $a(77) = 0.988 \pm 0.003$, while $a(273) = 1.037 \pm 0.003$; thus the direction of maximum resistivity changes from the c to the a direction as the temperature goes from 77 to 273 °K. This behavior is interpreted in terms of the resistivity anisotropy model of Klemens, Van Baarle, and Gorter, which is also used to qualitatively explain the observed anisotropies of the indium-lead alloys studied. Anomalies in the resistivity anisotropy were observed at 3.5- and 7.0 at. % lead, which were traced to anomalous behavior in the resistivity perpendicular to the c axis. The behavior at 7.0-at.% lead is interpreted as the Fermi surface popping through the (200) zone boundary. The temperature-dependent resistivity anisotropies of indium-lead alloys at 77 and 273 °K were determined, and at 273 °K, the direction of maximum temperature-dependent resistivity was found to change from the a to the c direction between 6- and 7-at. % lead. This behavior is attributed to an increasing perturbation of the indium lattice periodic potential by the lead ions at the relatively high temperature of 273 °K, and it is interpreted in terms of a breakdown in the δ-function potential approximation in the model of Klemens *et al.*

INTRODUCTION

Investigations in recent years on idium doped with lead have produced several interesting results in the 0–10-at. % region. These investigations have been concerned with superconducting transition temperature,[1,2] thermoelectric power,[3] electronic specific-heat coefficient,[2] and lattice spacings[4,5] of this system. If these various properties are plotted as a function of lead concentration, each will exhibit some interesting or "anomalous" behavior in the regions of 3.5- and 7.0-at. % lead, with the exception of the superconducting transition temperature which exhibits unusual behavior only near 7.0-at. % lead. These investigations gave impetus to the work reported here.

In the present investigation, nearly 100 cylindrical single-crystal specimens were prepared from pure indium and indium doped with 3–9 at. % lead. Approximately 80 of these specimens were considered to be of sample quality and had measurements made on them. Master alloys of 3.00-, 3.25-, 3.50-, 3.75-, 4.00-, 6.00-, 7.00-, 8.00-, and 9.00-at. % lead were prepared. A set of randomly oriented single-crystal samples was grown from each master alloy in addition to a set grown from pure indium.

The electrical resistivities along the cylindrical sample axis were measured at 4.2, 77, and 273 °K. In addition, the angle θ of the cystallographic c axis with respect to the cylindrical sample axis was determined for each sample. Since indium is tetragonal, the resistivity in a direction making an angle θ with the c axis can be written

$$\rho(\theta) = \rho_\perp + (\rho_\parallel - \rho_\perp)\cos^2\theta, \tag{1}$$

where $\rho_\parallel$ and $\rho_\perp$ are the resistivities parallel and perpendicular to the c axis. It is evident from Eq. (1) that a straight line drawn through the data for crystals of various orientations, plotted as ρ_{obs} versus $\cos^2\theta$, will yield $\rho_\parallel$ and $\rho_\perp$, and thus the resistivity anisotropy a, where $a \equiv \rho_\perp/\rho_\parallel$.

Although some work has been done on measuring the resistivities of pure indium[6–8] and indium doped with lead,[9–11] all of the previous work with the exception of that by Barisoni *et al.*[6] was done on polycrystalline samples and thus gives no direct measure of any anisotropies. We say "direct measure" because theoretical estimates of the anisotropy of the total resistivity can be made from polycrystalline data. For pure indium, Olsen[12] reported a value of 1.05 for the anisotropy at 273 °K. However, Olsen's value appears to have been a theoretical estimate based on polycrystalline data taken