FUNCTIONAL INTEGRAL APPROACH AND THE EIKONAL APPROXIMATION TO THE POLARON ENERGY AND MASS

Nhu Xuan Nguyen[1], Toan Thang Vu[2,*]

[1]*Faculty of Physics and Chemical Engineering, Le Quy Don Technical University, Hanoi, Vietnam*

[2]*Faculty of Basic Science, Ngo Quyen University, Binh Duong, Vietnam*

Abstract

This article uses the functional integral method and eikonal approximation to calculate the first-order correction for the energy and (effective) mass of the Polaron. The obtained results have demonstrated the effectiveness of the functional integral method compared to conventional perturbation theory when considering the Polaron problem in solid crystal.

Keywords: *Polaron problem; functional integral; eikonal approximation.*

1. Introduction

The polaron concept was first introduced by Lev Landau in 1933 [1] in his very short article [1], which was later developed by Solomon Pekar in 1946 [2], who studied the most basic properties of static polarons in the limiting case of very strong electron - phonon interactions. Many other famous researchers, including H. Frölich [3], R. Feynman [4, 5] and N. N. Bogolyubov [6]... then went on to contribute to the development of Polaron theory.

A polaron is a quasiparticle used in condensed matter physics to describe an electron moving in a dielectric crystal where the atoms displace from their equilibrium positions to effectively screen the charge of an electron, known as a phonon cloud. This lowers the electron mobility and increases the electron's effective mass. So it can be simply said that a Polaron is an electron "dressed" with its cloud of phonons and the properties of an electron wearing such a coat are in many cases completely different from the properties of a "bare" electron.

Various theoretical methods have been employed to approximate the polaron self-nergy and effective mass. They are all functions that depend on the Polaron interaction constant α [3].

The Polaron problem was first studied by Feynman [4] using the path-integral variational method and ordinary perturbation theory. With this method, he calculated the

* Email: vuthang76@gmail.com

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ground state energy and effective mass of Polaron [7] according to the weak interaction constant α (in the system $\hbar = c = 1$, α is a dimensionless constant).

$$E_0 = \frac{p^2}{2\mu_{\text{eff}}} - \alpha; \quad \mu_{eff} = \mu\left(1 + \frac{\alpha}{6}\right) \tag{1}$$

where μ is the electron mass, p is the initial momentum of the electron before interacting with the phonon.

For large α, Landau and Pekar [4] had pointed out

$$E_0 = \frac{p^2}{2\mu_{\text{eff}}} - a\alpha^2; \quad \mu_{eff} = \mu_0\left(1 + b\alpha^4\right) \tag{2}$$

where the constants a and b are determined phenomenologically in asymptotic form.

A few further refinements in the strong-coupling theories have also been worked out. However, calculating higher-order corrections for the above quantities is still difficult. Among the many methods of quantum field theory for this problem, the functional integration method appears to be an effective method. It has been used by many authors with many different approaches to calculate the correction energy and effective mass of Polaron [8]. The difficulty of this method is to encounter divergent integrals and accurately evaluate the integrals to calculate higher-order energy correction terms. To overcome this difficulty, we used the eikonal approximation to calculate the Feynman integrals of the Green function in the external field, which is a technique that is quite commonly used in the high-energy particle interaction problem of quantum field theory.

The purpose of this article is to use the eikonal approximation and the Feynman function integral method to calculate the ground state energy, its first-order energy correction, along with the effective mass of the Polaron. The outline of this article is organized as follows. In section 2, we will find the Green function of the polaron system in the crystal in the form of a general functional integral. Thanks to the eikonal approximation, we have linearized the Laplace operator from which we can find the Green function in the momentum representation. In the third section, we use the Green function obtained in Sec. 2 to find the ground state energy and first-order energy correction of the Polaron as well as find its effective mass. The discussion of the obtained results is presented in the last section.

2. The Green function of the polaron in the framework of functional integrals

For any interacting system in physics, the Green function is an important physical quantity because it describes the interactions of the system and allows us to find the basic physical quantities of the system such as energy, momentum, scattering amplitude...

In this section, we will find the Green function in representing the momentum of the polaron system in the form of functional integral based on solving the Schrodinger equation in the crystal lattice.

In the Fröhlich model of the Polaron, The Hamiltonian is determined by the sum of the free Hamiltonian H_o and the interaction Hamiltonian H_{int}, in which H_o includes the kinetic energy of the electron and the energy of the phonon and H_{int} is the interaction potential energy of these two types of particles† [8].

$$H = H_o + H_{\text{int}} = \left[\frac{1}{2\mu}\Delta_r + \frac{1}{2}\sum_k \omega_k \left(b_k^+ b_k + b_k b_k^+\right)\right] + \left[g\sum_k \left(A_k e^{i\vec{k}\vec{r}} b_k + A_k^* e^{-i\vec{k}\vec{r}} b_k^+\right)\right] \quad (3)$$

where b_k^+, b_k are the operators that create and annihilate phonons with wave vector $\vec{k}$ such that $\left[b_k^+, b_{k'}\right] = \delta_{kk'}$; ω_k is the lattice oscillation frequency; μ is the effective mass of the electron; Δ_r is the Laplace operator in coordinate representation; g is the lattice connection constant; A_k are the Fourier expansion coefficients of the current density.

Using the Bogoliubov canonical transformation, we substitute the following quantities into the Hamiltonian (3):

$$b_k \to \xi_k = e^{i\vec{k}\vec{r}} b_k; \quad b_k^+ \to \xi_k^+ = e^{-i\vec{k}\vec{r}} b_k^+; \quad -\mathrm{i}\vec{\nabla}_r \to \vec{P} - \sum_k \vec{k}\,\xi_k^+ \xi_k, \quad (4)$$

Hamiltonian (3) is rewritten as:

$$H = \frac{1}{2\mu}\left(\vec{P} - \sum_k \vec{k}\,\xi_k^+ \xi_k\right)^2 + \frac{1}{2}\sum_k \omega_k \left(\xi_k^+ \xi_k + \xi_k \xi_k^+\right) + g\sum_k \left(A_k \xi_k + A_k^* \xi_k^+\right) \quad (5)$$

The Green function of the polaron system corresponds to the Hamiltonian (5) in the momentum representation determined by the operator-form Schrodinger equation

$$\left(H - E\right).G = 1 \quad (6)$$

Using the inverse operator representation proposed by Fock-Feynman [9], we write

$$G = \frac{1}{H - E + i\varepsilon} = -i\int_0^\infty ds e^{i(H - E + i\varepsilon)s} = i\int_0^\infty ds e^{-i(E - i\varepsilon)s} G_s \quad (7)$$

where G_s is determined by‡

$$G_s = e^{iHs} = \exp\left\{\frac{is}{2\mu}\left(\vec{P} - \sum_k \vec{k}\,\xi_k^+ \xi_k\right)^2 + \frac{is}{2}\sum_k \omega_k \left(\xi_k^+ \xi_k + \xi_k \xi_k^+\right) + igs\sum_k \left(A_k \xi_k + A_k^* \xi_k^+\right)\right\} \quad (8)$$

† Use the atomic unit system $\hbar = c = 1$

‡ G_s satisfies the equation $-i\frac{\partial G_s}{\partial s} = HG_s; \quad G(s=0) = 1$

The Baker-Campbell-Hausdorff relation, $e^{A+B} = e^{A}.e^{B}.e^{-\frac{1}{2}[A,B]}$, is used to calculate the commutations in (8).

$$G_s = \exp\left\{\frac{is}{2}\sum_k \omega_k \left(\xi_k^+ \xi_k + \xi_k \xi_k^+\right)\right\}.g_s \tag{9}$$

where

$$\begin{aligned} g_s &= \exp\left\{\frac{is}{2\mu}\left(\vec{P} - \sum_k \vec{k}\xi_k^+ \xi_k\right)^2 + igs\sum_k \left[A_k \xi_k (1+\mathrm{is}\omega_k) + A_k^* \xi_k^+ (1-\mathrm{is}\omega_k)\right]\right\} \\ &\approx \exp\left\{\frac{is}{2\mu}\left(\vec{P} - \sum_k \vec{k}\xi_k^+ \xi_k\right)^2 + igs\sum_k \left[A_k \xi_k e^{\mathrm{is}\omega_k} + A_k^* \xi_k^+ e^{-\mathrm{is}\omega_k}\right]\right\} \end{aligned} \tag{10}$$

in (10), the approximation $e^x \approx 1+x$ has been used.

The exponential function of (10) is expressed in terms of *T*-product (Time-ordered product):

$$g_s = T\exp\left\{\frac{i}{2\mu}\int_0^s d\tau\left(\vec{P} - \sum_k \vec{k}\xi_k^+ \xi_k\right)^2 + ig\int_0^s d\tau\sum_k \left[A_k \xi_k e^{\mathrm{is}\omega_k} + A_k^* \xi_k^+ e^{-\mathrm{is}\omega_k}\right]\right\} \tag{11}$$

In (11), expressions in exponential functions that have non-commutative quantities such as $\xi_k(\tau), \omega_k(\tau)$ according to Feynman are considered T_ξ-exponent. The variable τ has the meaning of a proper time divided by the mass of the particle and plays the role of *T*-product in (11). The subscript *s* means proper time. All operators are considered commutative functions of the variable τ.

The first term of (11) is a quadratic function according to the differential operator, so we can represent it as a product of lower order operators by using the Weierstrass transformation [10] in the 4-dimensional function space as follows:

$$\begin{aligned} &\exp\left\{\int_0^s A_\tau^2 d\tau\right\} = \exp\left\{\int_0^s d\tau\left[\left(\vec{A}_\tau^2 + \vec{v}^2(\tau) - 2\vec{v}(\tau)\vec{A}_\tau\right) - \left(\vec{v}^2(\tau) - 2\vec{v}(\tau)\vec{A}_\tau\right)\right]\right\} \\ &= C.\exp\left\{-\int_0^s d\tau.\vec{v}^2(\tau)\right\}.\exp\left\{2\int_0^s d\tau.\vec{v}(\tau)\vec{A}_\tau\right\} = \int\left[\delta\vec{v}\right]_0^s.\exp\left\{2\int_0^s d\tau.\vec{v}(\tau)\vec{A}_\tau\right\} \end{aligned} \tag{12}$$

where $A_s^2 = \frac{1}{2\mu}\left(\vec{P} - \sum_k \vec{k}\xi_k^+ \xi_k\right)^2$.

The functional integral is expanded on the 4-dimensional function space $\nu(\tau)$ according to the Gauss measure, the C-constant is determined by the condition:

$$C\int \delta\vec{\nu}\exp\left\{-i\int_0^s \vec{\nu}^2(\tau)d\tau\right\}=1 \tag{13}$$

and

$$\left[\delta\vec{\nu}(\tau)\right]_0^s=\frac{\delta\vec{\nu}\exp\left\{-i\int_0^s \vec{\nu}^2(\tau)d\tau\right\}}{\int \delta\vec{\nu}\exp\left\{-i\int_0^s \vec{\nu}^2(\tau)d\tau\right\}} \tag{14}$$

is a volume element of the functional space of the 4-dimensional function defined on the interval $0\le\tau\le s$ [10].

The functional variables $\nu(\tau)$ formally introduced for obtaining the solution of the Green function describe the deviation of a particle trajectory from the straight-line paths. The functional with respect to $\left[\delta\vec{\nu}(\tau)\right]$ corresponds to the summation over all possible trajectories of the colliding particles [10].

The expression (11) become:

$$g_s=\int\left[\delta\vec{\nu}(\tau)\right]_0^\tau \exp\left(i\sqrt{\frac{2}{\mu}}\int_0^s d\tau\vec{\nu}(\tau).\vec{P}\right).f(\vec{\nu}) \ , \tag{15}$$

where $f(\vec{\nu})$ is determined by

$$f(\vec{\nu})=T\exp\left[-i\sqrt{\frac{2}{\mu}}\int_0^s d\tau\vec{\nu}(\tau).\sum_k \vec{k}\xi_k^+\xi_k+ig\int_0^s d\tau\sum_k\left(A_k\xi_k e^{\mathrm{is}\omega_k}+A_k^*\xi_k^+e^{-\mathrm{is}\omega_k}\right)\right] \tag{16}$$

Debug the operator according to Feynman's rule and use the following displacement formula $e^{\varphi_\mu\partial_\mu}f(x)=f(x+\varphi_\mu)$ [10], (16) is expressed as a functional integral

$$\begin{aligned} f(\vec{\nu})&=\exp\left[-i\sqrt{\frac{2}{\mu}}\int_0^s d\tau\vec{\nu}(\tau).\sum_k \vec{k}\xi_k^+\xi_k\right].\\ &.\exp\left[ig\sum_k A_k^*\xi_k^+\int_0^s d\tau e^{-\mathrm{i}\int_0^\tau d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{\nu}(\tau)\right)}\right].\exp\left[ig\sum_k A_k\xi_k\int_0^s d\tau e^{\mathrm{i}\int_0^\tau d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{\nu}(\tau)\right)}\right] \end{aligned} \tag{17}$$

Substitute (17) into (15) and (9), the final expression for the Green function of the Polaron in the crystal is obtained as follows:

$$G = i\int_0^\infty ds e^{-i(E-i\varepsilon)s} \exp\left\{\frac{is}{2}\sum_k \omega_k\left(\xi_k^+\xi_k + \xi_k\xi_k^+\right)\right\}$$
$$\times\int\left[\delta\vec{v}(\tau)\right]_0^\tau \exp\left(i\sqrt{\frac{2}{\mu}}\int_0^s d\tau\vec{v}(\tau)\vec{P}\right).\exp\left[-i\sqrt{\frac{2}{\mu}}\int_0^s d\tau\vec{v}(\tau).\sum_k \vec{k}\xi_k^+\xi_k\right]$$
$$\times\exp\left[ig\sum_k A_k^*\xi_k^+\int_0^s d\tau e^{-i\int_0^\tau d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)}\right].\exp\left[ig\sum_k A_k\xi_k\int_0^s d\tau e^{i\int_0^\tau d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)}\right] \quad (18)$$
$$\times\exp\left[-g^2\sum_k|A_k|^2\int_0^s d\tau_1 e^{i\int_0^{\tau_1} d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)}.\int_0^{\tau_1} d\tau_2 e^{i\int_0^{\tau_2} d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)}\right]$$

We will study processes whose initial and final states do not have free quanta. Then, the vacuum mean value of Green's function takes the form:

$$\langle 0|G|0\rangle \equiv G_0(s) = i\int_0^\infty ds e^{-i(E-i\varepsilon)s}.\int\left[\delta\vec{v}(\tau)\right]_0^\tau \exp\left(i\sqrt{\frac{2}{\mu}}\int_0^s d\tau\vec{v}(\tau)\vec{P}\right)$$
$$\times\exp\left[-g^2\sum_k|A_k|^2\int_0^s d\tau_1 e^{i\int_0^{\tau_1} d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)}.\int_0^{\tau_1} d\tau_2 e^{i\int_0^{\tau_2} d\eta\left(\omega_k-\sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)}\right] \quad (19)$$

Note that

$$G_0(s) = \langle 0|e^{-sH}|0\rangle = \sum_n \langle 0|e^{-sH}|\varphi_n\rangle\langle\varphi_n|0\rangle = \sum_n e^{-sE_n}|\langle\varphi_n|0\rangle|^2$$
$$= e^{-sE_0}\left[|\langle\varphi_n|0\rangle|^2 + \sum_{n\neq 0} e^{-s(E_n-E_0)}|\langle\varphi_n|0\rangle|^2\right] \quad (20)$$
$$\Rightarrow G_0(s) \to e^{-sE_0}.|\langle\varphi_n|0\rangle|^2$$

where $E_0 \equiv E_0(\vec{P})$ is the basic energy level of the system given the momentum $\vec{P}$, $|0\rangle$ is the vacuum state of the system without taking into account interactions, $|\varphi_n\rangle$ is the complete set of states of the Hamiltonian operator *H* with energy E_n.

In the next section, we will use the expression of Green's function (19) to find the energy in the ground state and the first-order correction for the energy along with the effective mass of the Polaron in the case of weak bond and medium strong bond.

3. The first-order correction for the energy spectrum and the effective mass of the Polaron

In this section, the Green function in the straightline path approximation will be used to deduce the expression for the energy in quantum states. Performing calculations in the limit cases where the electron momentum is large and small, we will find the effective mass of the Polaron and the first-order corrections for the energy in the cases of weak bond and medium strong bond.

3.1. The vacuum expectation of the Green's function in the eikonal approximation

To calculate the vacuum expectation value for the Green function according to expression (19), we will perform a series of complex functional transformations and use the properties of the eikonal approximation. The first is to perform functional transformation

$$\vec{v}(\tau) \to \vec{v}(\tau) + \frac{\vec{P}}{\sqrt{2\mu}} \tag{21}$$

and change the order of integration, then (19) becomes:

$$\begin{aligned} \langle 0|G|0\rangle &= i\int_0^\infty ds e^{-is\left(E-\frac{P^2}{2\mu}-i\varepsilon\right)} .\int \left[\delta\vec{v}(\tau)\right]_0^\tau \\ &\times \exp\left\{-g^2\sum_k |A_k|^2 \int_0^s d\tau_1 .\int_0^{\tau_1} d\tau_2 e^{i\int_0^{\tau_2} d\eta\left(\omega_k - \sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)} \exp\left[i\int_{\tau_2}^{\tau_1} d\eta\left(\omega_k - \sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta) - \frac{\vec{k}\vec{P}}{\mu}\right)\right]\right\} \end{aligned} \tag{22}$$

In (22), Gaussian integration was used:

$$\int \left[\delta\vec{v}(\tau)\right]_0^\tau \exp\left(i\sqrt{\frac{2}{\mu}}\int_0^s d\tau \vec{v}(\tau)\vec{P}\right) = i\frac{P^2}{2\mu}\int \left[\delta\vec{v}(\tau)\right]_0^\tau \tag{23}$$

and continue to use the following eikonal approximation

$$\begin{aligned} &\bar{\pi}[\vec{v}(\tau)] = \int \left[\delta\vec{v}(\tau)\right]_0^\tau .\bar{\pi}[\vec{v}(\tau)], \\ &\int \left[\delta\vec{v}(\tau)\right]_0^\tau .\exp\left(F(\vec{v})\right) \approx \exp \bar{F}(\vec{v}) = \exp \int \left[\delta\vec{v}(\tau)\right]_0^\tau .F(\vec{v}) \end{aligned} \tag{24}$$

We set

$$\begin{aligned} F(\vec{v}) &= -g^2\sum_k |A_k|^2 \int_0^s d\tau_1 .\int_0^{\tau_1} d\tau_2 e^{i\int_0^{\tau_2} d\eta\left(\omega_k - \sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta)\right)} \exp\left[i\int_{\tau_2}^{\tau_1} d\eta\left(\omega_k - \sqrt{\frac{2}{\mu}}\vec{k}\vec{v}(\eta) - \frac{\vec{k}\vec{P}}{\mu}\right)\right], \\ &= -g^2\sum_k |A_k|^2 \int_0^s d\tau_1 .\int_0^{\tau_1} d\tau_2 \exp\left[i\left(\omega_k - \frac{\vec{k}\vec{P}}{\mu}\right)(\tau_1 - \tau_2)\right] \exp\left[-i\sqrt{\frac{2}{\mu}}\vec{k}\int_{\tau_2}^{\tau_1} d\eta \vec{v}(\eta)\right] \end{aligned} \tag{25}$$

to calculate $\int\left[\delta\vec{v}(\tau)\right]_0^{\tau}.F(\vec{v})$ by using (23) and (24). The vacuum mean value of the Green function is

$$\begin{aligned}\left\langle 0\middle|G\middle|0\right\rangle &= i\int_0^{\infty} ds e^{-is\left(E-\frac{P^2}{2\mu}-i\varepsilon\right)}\times \\ &\exp\left\{-g^2\sum_k\left|A_k\right|^2\int_0^s d\tau_1.\int_0^{\tau_1}d\tau_2\exp\left[i\left(\omega_k-\frac{1}{\mu}\vec{k}.\vec{P}+\frac{1}{2\mu}k^2\right)(\tau_1-\tau_2)\right]\right\}\end{aligned} \tag{26}$$

Setting $\Omega_k=\omega_k-\frac{1}{\mu}\vec{k}.\vec{P}+\frac{1}{2\mu}k^2$ (Polaron effective frequencies), then, integrating over the variables τ_2,τ_1 and *s*, we obtain the final expression of Green's function

$$\begin{aligned}\left\langle 0\middle|G\middle|0\right\rangle &= i\int_0^{\infty} ds e^{-is\left(E-\frac{P^2}{2\mu}-i\varepsilon\right)}\times\exp\left[g^2\sum_k\frac{\left|A_k\right|^2}{\Omega_k}\left(e^{is\Omega_k}-is\Omega_k-1\right)\right] \\ &= \sum_{n_k}P_{(n_k)}\frac{1}{E-\frac{P^2}{2\mu}-g^2\sum_k\frac{\left|A_k\right|^2}{\Omega_k}-\sum_k n_k\Omega_k-i\varepsilon}\end{aligned} \tag{27}$$

where $P_{(n_k)}a$ is the Poisson probability, n_k are positive integers indicating the energy state index.

$$P_{(n_k)}=\prod_k e^{-\bar{n}_k}\frac{(\bar{n}_k)^{n_k}}{n_k!};\quad \bar{n}_k=g^2\frac{\left|A_k\right|^2}{\Omega_k^2} \tag{28}$$

From (27), expression of the Polaron energy is derived (singularity of Green's function)

$$E=\frac{P^2}{2\mu}+g^2\sum_k\frac{\left|A_k\right|^2}{\Omega_k}+\sum_k n_k\Omega_k \tag{29}$$

In the expression of Ω_k, there is an additional term $\frac{1}{2\mu}k^2$, which means that in the eikonal approximation the recoil of the particles when interacting with the field is included. However, this effect only takes into account the elastic interaction with the recoil particle's momentum equal to the forward particle's momentum, not taking into account that these momentums are different. This will be a problem that we will continue to consider in the future.

3.2. Ground state energy and effective mass of Polaron

In the Fröhlich model of the Polaron, particle interactions in the periodic field of the ionic lattice were considered [8]. Using perturbation theory for this model one has

$$gA_k = -\frac{ie}{|\vec{k}|}\sqrt{\frac{2\pi\omega_k a_k}{V}} \tag{30}$$

where e is the electron charge, V is the system volume, ω_k are lattce vibrations, a_k are dimensioness constants.

In the ground state, we set $n_k = 0$ into (29) and assume that ω_k and a_k do not depend on k, and also consider that the system volume is very large to switch from summation to integration over the particle's momentum, $\frac{1}{V}\sum_k ... \to \frac{1}{(2\pi)^3}\int d\vec{k}$, we have

$$\begin{aligned} E_0 &= \frac{P^2}{2\mu} - \frac{2\pi\omega a}{V}\sum_k \frac{1}{\Omega_k}\frac{e^2}{|\vec{k}|^2} \\ \to E_0 &= \frac{P^2}{2\mu} - \frac{e^2\omega a}{(2\pi)^2}\int d\vec{k}\,\frac{1}{\vec{k}^2}.\frac{1}{\Omega_k} = \frac{P^2}{2\mu} - \frac{2\mu e^2\omega a}{(2\pi)^2}\int d\vec{k}\,\frac{1}{\vec{k}^2\left(\vec{k}^2 + 2\mu\omega - 2\vec{k}\vec{P}\right)} \end{aligned} \tag{31}$$

The following integration formula has been applied to (31)

$$\frac{1}{\alpha_1\alpha_2} = \int_0^1 dx \frac{1}{\left[\alpha_1 x - \alpha_2(1-x)\right]^2} \tag{32}$$

then

$$E_0 = \frac{P^2}{2\mu} - \frac{2\mu e^2\omega a}{(2\pi)^2}\int_0^1 dx \int \frac{d\vec{k}}{\left[\vec{k}^2 + 2\mu\omega(1-x) - \vec{P}^2(1-x)^2\right]^2}. \tag{33}$$

to introduce the dimensioness constants

$$\theta^2 = \frac{\vec{P}^2}{2\mu\omega}, \quad \lambda = ae^2\sqrt{\frac{\mu}{2\omega}}, \tag{34}$$

and use Feynman integration

$$\int \frac{d^3k}{(2\pi)^3}\frac{1}{(k^2 + a^2)} = \frac{1}{8\pi\sqrt{a}}, \tag{35}$$

The expression for ground state energy is obtained

$$E_0 = \theta^2\omega - \lambda\omega f(\theta), \tag{36}$$

where

$$f(\theta) = \frac{1}{2}\int_0^1 \frac{dx}{\sqrt{x(1-\theta^2 x)}} = \begin{cases} \dfrac{1}{\theta}\arcsin\theta & \text{if } \theta<1 \\ \dfrac{1}{\theta}\left(\dfrac{\pi}{2}\text{-}\arccos\theta\right) & \text{if } \theta>1 \end{cases} \tag{37}$$

We consider two limited regions when θ is small and θ is large.

• When θ is small then $f(\theta) \approx 1 + \frac{1}{6}\theta^2$. Substituting $f(\theta)$ into (33) yields

$$E_0 = \theta^2\omega - \lambda\omega - \frac{1}{6}\lambda\omega\theta^2 = \varepsilon + \frac{\vec{P}^2}{2\mu_{eff}}, \tag{38}$$

where $\varepsilon = -\lambda\omega$ and $\mu_{eff} = \dfrac{\mu}{\left(1-\frac{1}{6}\lambda\right)} \approx \mu\left(1+\frac{1}{6}\lambda\right)$.

This result completely coincides with the results obtained from perturbation theory [4].

• In the opposite case, when θ is large, the expression $f(\theta)$ is in asymptotic form $f(\theta) \approx \frac{1}{\theta}\left[\frac{\pi}{2} + i\ln(2\theta) + O\left(\frac{1}{\theta^2}\right)\right]$ and we have

$$E_0 = \omega\theta^2 - \frac{\lambda\omega}{\theta}\left[\frac{\pi}{2} + i\ln(2\theta)\right] + O\left(\frac{1}{\theta^3}\right), \tag{39}$$

3.3. First-order correction for the energy in the ground state of the Polaron system

To calculate the first-order correction for the energy in the gound state based on the eikonal approximation, we must retain the interaction terms k_i, k_j ($i \neq j$), which are related to the interaction between particles and the quantum of the field. This correlation contribution is expressed according to the following expansion

$$\int\left[\delta\vec{v}(\tau)\right]_0^{\tau}.\exp\left\{F(\vec{v})\right\} = \exp\left[\bar{F}(\vec{v}) - \frac{1}{4}\int ds\left(\frac{\delta\bar{F}(\vec{v})}{\delta\vec{v}(\tau)}\right)^2 + \ldots\right], \tag{40}$$

where $F(\vec{v})$ is determined by (25).

The first term in (25) was calculated based on approximation (24). The second term will be determined as follows:

$$\frac{\delta\bar{F}(\vec{v})}{\delta v(\tau)} = \int[\delta v(\tau)]\frac{\delta F(\vec{v})}{\delta v(\tau)} = -g^2\sum_k |A_k|^2 \int_0^s d\tau_1 . \int_0^{\tau_1} d\tau_2 \exp\left[i\left(\omega_k - \frac{\vec{k}\vec{P}}{\mu} \right)(\tau_1 - \tau_2) \right] \times \int[\delta v(\tau)]\frac{\delta F(\vec{v})}{\delta v(\tau)} \exp\left[-i\sqrt{\frac{2}{\mu}}\vec{k}\int_{\tau_2}^{\tau_1} d\eta \vec{v}(\eta) \right] \tag{41}$$

$$\frac{\delta\bar{F}(\vec{v})}{\delta v(\tau)} = -ig^2\sqrt{\frac{2}{\mu}}\sum_k \vec{k}|A_k|^2 \int_0^s d\tau_1 . \int_0^{\tau_1} d\tau_2 \exp\left[i\Omega_k(\tau_1 - \tau_2) \right] \tag{42}$$

where Ω_k has been defined in (26).

Performing integration over the variables, we get

$$\frac{\delta\bar{F}(\vec{v})}{\delta v(\tau)} = -ig^2\sqrt{\frac{2}{\mu}}\sum_k \vec{k}|A_k|^2 \frac{1}{\Omega_k^2}\left[i\Omega_k s - e^{i\Omega_k s} + 1 \right] \tag{43}$$

then

$$\delta E_0 = -\frac{1}{4}\int ds\left(\frac{\delta\bar{F}}{\delta\vec{v}(\tau)} \right)^2 = \frac{1}{2\mu}\left[g^2\sum_k \vec{k}|A_k|^2 \frac{1}{\Omega_k^2} \right]^2 \left[i\Omega_k s - e^{i\Omega_k s} + 1 \right]^2 s \approx \frac{1}{2\mu}\left[g^2\sum_k \vec{k}|A_k|^2 \frac{1}{\Omega_k^2} \right]^2 s = \frac{1}{2\mu}\eta^2\vec{P}^2 = \omega\eta^2\theta^2 \tag{44}$$

In (44), we have approximated to the first order term. The parameter a is determined from the condition

$$g^2\sum_k \vec{k}|A_k|^2 \frac{1}{\Omega_k^2} = \eta\vec{P}, \tag{45}$$

From (45), we see that the condition for applying the eikonal approximation is η <<1, i.e. the sum over momentum $\vec{k}$ must converge. Comparing with expressions (36) and (37), we deduce the value of parameter η is

$$\eta = \frac{\lambda}{2\theta} f'(\theta) = \begin{cases} \dfrac{\lambda}{6} & \text{if } \theta<1 \\ -\dfrac{i\lambda}{2\theta^3}\ln(2\theta) & \text{if } \theta>1 \end{cases} \tag{46}$$

Substitute (46) into (44) to obtain the expression of the first-order correction for the ground state energy

$$\delta E_0 = \begin{cases} \omega \dfrac{\lambda^2 \theta^2}{36} & \text{if } \theta<1 \\ -\omega \dfrac{\lambda^2}{4\theta^4} \ln^2(2\theta) & \text{if } \theta>1 \end{cases} \quad (47)$$

From the condition to apply the eikonal approximation of η <<1, we see:

- For slow particles (i.e. θ << 1) the condition is λ << 1, this case describes the polarization state of the particle when interacting with the field, it corresponds to the "weak coupling" of the particle with the field.

- For fast particles (i.e. θ >> 1) the condition is $\dfrac{\lambda \ln(2\theta)}{\theta^3}$ << 1, which corresponds to the "moderately strong coupling" of the particle with the field.

Higher order approximations to the ground state energy can show that the ground state energy of the Polaron can be expressed as

$$E_0 = \omega\theta^2 - \lambda\omega \sum_{n=0} (\lambda\theta^2) f_n(\theta) \quad (48)$$

where $f_n(\theta)$ is a regular function, receiving a non-zero constant value when θ = 0.

4. Conclusion

To summarize, the functional integration method and the eikonal approximation have been effectively used to determine the energy in the ground state and its first correction as well as calculate the effective mass of the Polaron when electrons interact with the crystal field. In addition to basic results that coincide with the results obtained by many previous authors using other methods, we have calculated the first-order correction term and generalized it to the higher-order term.

There exists an enomours amount of literature on the subject of the "polaron mass". A large group publication is concerned with direct pertubational or variational treatment of the Hamiltonian. We find excellent agreement for small θ, in intermediate and middle strong-coupling. The functional integral bounds are systematically lower than all others, leading to the conclusion that this method is more adequate. It is well known that many authors used functional integral methods before us in polaron physics. However, we still use that method because it is one of the few places where path integration not only helps you find the answer but is also the best way to calculate the answer even if you already have it.

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CÁCH TIẾP CẬN TÍCH PHÂN PHIẾM HÀM VÀ PHÉP GẦN ĐÚNG EIKONAL KHI TÍNH TOÁN NĂNG LƯỢNG VÀ KHỐI LƯỢNG POLARON

Nguyễn Như Xuân[1], Vũ Toàn Thắng[2]

[1]*Khoa Hóa - Lý kỹ thuật, Trường Đại học Kỹ thuật Lê Quý Đôn, Hà Nội, Việt Nam*

[2]*Khoa Cơ bản, Trường Đại học Ngô Quyền, Bình Dương, Việt Nam*

Tóm tắt: Bài báo sử dụng phương pháp tích phân phiếm hàm và phép gần đúng eikonal để tính toán bổ chính bậc nhất cho năng lượng và khối lượng (hiệu dụng) của Polaron. Các kết quả thu được đã chứng tỏ sự hữu hiệu của phương pháp tích phân phiếm hàm so với lý thuyết nhiễu loạn thông thường khi xem xét bài toán Polaron trong vật rắn.

Từ khóa: *Bài toán Polaron; tích phân phiếm hàm; gần đúng eikonal.*

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