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Particles and shadows: a generalized path-integral approach to non-relativistic field theories

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Abstract. Luttinger and Lu have derived a variational method for representing the Yukawa interaction of bosons and fermions in non-relativistic field theories by a general potential between fermions and fictitious particles ('shadows'). In the present work, this is considerably improved by applying Jensen's inequality only once and representing the kinetic term in the path-integral average as a quantum-mechanical N-body problem using the replica technique. Various weak- and strong-coupling approximations as well as variational bounds for this term are discussed.

1. Introduction

Many non-relativistic systems in solid state and nuclear physics can be described by field-theoretical models of fermions interacting with bosons. The Hamiltonian of such a system of A fermions with mass m usually has the form

$$\hat{H} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \int \mathrm{d}^3k\, \omega(k) a^\dagger(k) a(k) + \sqrt{\alpha} \sum_{i=1}^{A} \int \frac{\mathrm{d}^3k}{(2\pi)^3} [f(k) a^\dagger(k) \mathrm{e}^{-\mathrm{i}k\cdot x_i} + \mathrm{HC}] \tag{1}$$

when the interaction is assumed to be spin-independent. Here $a(k)$ and $a^\dagger(k)$ are annihilation and creation operators for the bosons (phonons or mesons), $\omega(k)$ denotes the boson frequency and α is a dimensionless coupling constant between fermions and bosons. For the well known polaron problem [1–4], the function $f(k)$ is given by

$$f(k) = \mathrm{i} \left(\frac{4\pi}{\sqrt{2}} \right)^{1/2} \frac{1}{|k|}. \tag{2}$$

For the meson–nucleon problem see [5, 6]. In the following I will only consider the zero-momentum self-energy of a single fermion ($A = 1$) interacting with any number of bosons.

Feynman [7] observed that the bosons can be eliminated analytically since they enter, at most, quadratically in the Hamiltonian (1). In the path-integral formulation, one obtains an effective action for the fermion which, for large Euclidean time β, is given by

$$S = \int_0^\beta \mathrm{d}t\, \frac{m}{2} \dot{x}^2 - \alpha \int_0^\beta \mathrm{d}t \int_0^\beta \mathrm{d}t' \int \frac{\mathrm{d}^3k}{(2\pi)^3} |f(k)|^2 \mathrm{e}^{-\omega(k)|t-t'|} \mathrm{e}^{\mathrm{i}k\cdot(x(t)-x(t'))} \equiv S_0 + S_1. \tag{3}$$

With the elimination of the bosonic degrees of freedom, one is left with a one-body effective theory which, however, is highly non-local in time due to the retardation effects. This

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prevents a Hamiltonian formulation and any further exact analytical treatment. Instead, Feynman used a variational formulation for the partition function

$$Z = \int_{x(0)=x(\beta)} \mathcal{D}[x] e^{-S[x]} \tag{4}$$

based on Jensen's inequality $\langle \exp(-S) \rangle \geqslant \exp(-\langle S \rangle)$. This yields an upper limit for the ground-state energy (self-energy at zero momentum)

$$E_0 \leqslant E_{\text{trial}} + \lim_{\beta\to\infty} \frac{1}{\beta} \langle S - S_{\text{trial}} \rangle_{S_{\text{trial}}} \tag{5}$$

where E_{trial} is the energy corresponding to some suitably chosen trial action S_{trial} and the average is performed with respect to S_{trial}.

The trial action proposed by Feynman for the polaron problem is that of a retarded harmonic oscillator and in the usual polaron units ($m = \omega = 1$) it is given by

$$S_F = \int_0^\beta d\tau \frac{1}{2}\dot{x}^2 + \frac{w}{4}(v^2 - w^2) \int_0^\beta d\tau \int_0^\tau d\tau' e^{-w(\tau-\tau')} |x(\tau) - x(\tau')|^2 \tag{6}$$

where v and w are variational parameters. They are determined by minimizing equation (5) which becomes

$$E_0 \leqslant E_F = \frac{3}{4v}(v-w)^2 - \frac{v\alpha}{\sqrt{\pi}} \int_0^\infty d\tau \frac{e^{-\tau}}{[w^2\tau + (v^2-w^2)(1-e^{-v\tau})/v]^{1/2}}. \tag{7}$$

Feynman's approach is the best analytical approximation which works for both weak and strong coupling. Recent precise Monte Carlo calculations [8] indicate that the maximal error occurs for large α; from the known strong-coupling expansions, one may then estimate that the Feynman ground-state energy deviates less than 2.2% from the exact value in the whole range of coupling constants.

2. Luttinger and Lu's approach and improvement

The ansatz (6) was motivated [7, 9] by the fact that it results from 'integrating out' a fictitious particle with mass

$$M = \frac{v^2 - w^2}{w^2} \tag{8a}$$

and coordinate $\boldsymbol{R}$ which couples *harmonically* to the electron

$$V(\boldsymbol{R} - \boldsymbol{x}) = \tfrac{1}{2} M w^2 (\boldsymbol{R} - \boldsymbol{x})^2. \tag{8b}$$

This 'shadow' particle simulates the cloud of phonons around the electron in the crystal.

Luttinger and Lu (LL) [10] have generalized this idea to an arbitrary potential $V(\boldsymbol{R} - \boldsymbol{x})$ and have shown that for large coupling constants the best effective potential is not harmonic (as in Feynman's approximation) but Coulomb-like. In this way, they obtained the exact

strong-coupling limit for the ground-state energy due to Pekar [11] and Miyake [12]. Their method is based on multiplying equation (4) by

$$1 = \frac{\int \mathcal{D}[\boldsymbol{R}] \exp(-T[\boldsymbol{R}-\boldsymbol{x}] + T_1[\boldsymbol{R}-\boldsymbol{x}])}{\int \mathcal{D}[\boldsymbol{R}] \exp(-T_0[\boldsymbol{R}])} \tag{9}$$

where

$$T[\boldsymbol{R}-\boldsymbol{x}] = \int_0^\beta \mathrm{d}t \left(\frac{M}{2}\dot{\boldsymbol{R}}^2 + V(\boldsymbol{R}-\boldsymbol{x})\right) \equiv T_0[\boldsymbol{R}] + T_1[\boldsymbol{R}-\boldsymbol{x}] \tag{10}$$

is the action of a shadow particle coupled to the fermion. They then invoked again Jensen's inequality for the combined-path integral and determined the optimal-potential function $V(r)$ and mass parameter M. An important observation made by LL is that the non-Gaussian path integrals, which necessarily occur in their approach, can be evaluated by solving the corresponding quantum-mechanical problem (i.e. the Schrödinger equation). For example

$$\int \mathcal{D}[\boldsymbol{x}]\mathcal{D}[\boldsymbol{R}] \exp(-S_0[\boldsymbol{x}] - T[\boldsymbol{R}-\boldsymbol{x}]) = \text{constant} \times \mathrm{Tr}(\mathrm{e}^{-\beta \hat{H}_2}) \tag{11a}$$

where

$$\hat{H}_2 = \frac{\boldsymbol{P}^2}{2(M+m)} + \frac{\boldsymbol{p}^2}{2\mu} + V(r) \tag{12}$$

is the two-body Hamiltonian in centre-of-mass and relative coordinates with reduced mass $\mu = mM/(M+m)$.

However, applying the inequality *twice*, i.e. to particle *and* shadow, leads to a bad approximation except for large coupling constants. This is best seen for a harmonic interaction where LL obtain nearly the same result (7) as Feynman but with the first term (which I will call the 'kinetic' part) being replaced by $3v/4$. This leads to much more repulsion at small α: instead of Feynman's $(v-w)^2/v = \mathcal{O}(\alpha^2)$ LL only have $v = \mathcal{O}(1)$. The difference does not matter at large coupling constants when $v \gg w$ but is essential at low and intermediate coupling. As a consequence, E_{LL} (in the so-called ground-state approximation) is only better than E_{F} for $\alpha > 34$ despite the fact that an arbitrary potential $V(r)$ has been allowed for the variational principle. This basically renders the LL approach a complicated strong-coupling expansion.

To improve the LL treatment and to exploit the full flexibility of a general potential, it seems necessary to use Jensen's inequality only *once*. This can be accomplished by defining the trial action directly as a result of the elimination of a shadow particle

$$\exp(-S_{\mathrm{trial}}[\boldsymbol{x}]) = \int \mathcal{D}[\boldsymbol{R}] \exp(-S_0[\boldsymbol{x}] - T[\boldsymbol{R}-\boldsymbol{x}]). \tag{13}$$

Note that this is translationally invariant and reduces to Feynman's ansatz (6) for a harmonic interaction. One then has to evaluate the individual averages in equation (5).

The simplest term is the trial energy E_{trial}: using equation (11a) one immediately obtains

$$E_{\mathrm{trial}} = \epsilon_0^{(2)} \tag{14}$$

where $\epsilon_0^{(2)}$ (I suppress the superscript in most of the following) is the lowest eigenvalue of the two-body Hamiltonian (12). Note that, after separation of the centre-of-mass motion,

this reduces to the determination of the lowest energy of a particle of mass μ in an (up to now) arbitrary potential $V(r)$—a problem which can be solved easily by standard numerical methods.

The evaluation of $\langle S_1\rangle_{S_{\rm trial}}$ proceeds similarly using the equivalence

$$\int \mathcal{D}[x]\mathcal{D}[R]\mathcal{O}_1(t_1)\mathcal{O}_2(t_2)\exp(-S_0[x]-T[R-x])$$

$$= \text{constant}\times \mathrm{Tr}(\mathcal{T}\hat{\mathcal{O}}_{1\mathrm{H}}(t_1)\hat{\mathcal{O}}_{2\mathrm{H}}(t_2)\mathrm{e}^{-\beta\hat{H}_2}) \tag{11b}$$

where $\mathcal{T}$ is the time-ordering symbol and $\hat{\mathcal{O}}_{\mathrm{H}}(t)$ denotes the corresponding Heisenberg operator. A straightforward evaluation yields the same expression as that given by LL

$$\langle S_1\rangle_{S_{\rm trial}} = -\alpha\int\frac{\mathrm{d}^3k}{(2\pi)^3}|f(k)|^2\sum_n\frac{|\langle 0|\exp(\mathrm{i}\mu k\cdot r/m)|n\rangle|^2}{\omega(k)+\epsilon_n-\epsilon_0+k^2/2(M+m)}. \tag{15}$$

Note that here knowledge of the full spectrum of $\hat{H}_2$ is needed which makes the numerical evaluation of equation (15) for a general potential a major task. However, as observed by LL, each term in the spectral sum gives a positive contribution so that one still has an upper bound on the energy if only a finite number of states are retained. In the strong-coupling limit the ground-state contribution already leads to the exact Pekar result.

The last average to be evaluated is $\langle S_0 - S_{\rm trial}\rangle_{S_{\rm trial}}$. Although this is nearly trivial for a harmonic interaction, i.e. in Feynman's approximation†, it turns out to be the most challenging problem for a general potential and it is the major topic of this work. This is due to the fact that the trial action $S_{\rm trial}$ appears directly for the first time and not only in the form $\exp(-S_{\rm trial})$ in which it can readily be transformed into quantum-mechanical expectation values as in equations (11). Using definition (13) for the trial action, an alternative formulation of the problem is to evaluate the non-standard path integral

$$\langle S_0-S_{\rm trial}\rangle_{S_{\rm trial}} = \int\mathcal{D}[x]\mathcal{D}[R]\exp(-S_0[x]-T[R-x])\log\left[\int\mathcal{D}[R_1]\exp(-T[R_1-x])\right]$$

$$\times\left(\int\mathcal{D}[x]\mathcal{D}[R]\exp(-S_0[x]-T[R-x])\right)^{-1}. \tag{16}$$

3. Replicas

Obviously it is the logarithm in equation (16) which prevents a formulation in terms of stationary quantum mechanics as in the previous terms. A similar problem arises in the linked-cluster theorem which states that $\log Z$ is given by the sum of connected diagrams. An elegant method to prove this theorem is the *replica* technique [13] based on the representation

$$\log Z = \lim_{N\to 0}\frac{\partial}{\partial N}Z^N. \tag{17}$$

† In particular, if the Fourier path-integral form is used [8].

For integer N, Z^N can again be represented as a quantum-mechanical expectation value with a Hamiltonian containing N 'replicas' of the original particles. Applying this trick to the evaluation of $\langle S_0 - S_{\text{trial}}\rangle$, one obtains, after renumbering $N \to N+1$,

$$\langle S_0 - S_{\text{trial}}\rangle_{S_{\text{trial}}} = \frac{\partial}{\partial N}\,\text{Tr}(e^{-\beta \hat{H}_{N+1}})\bigg|_{N=1} \tag{18}$$

where the $(N+1)$-body Hamiltonian is given by

$$\hat{H}_{N+1} = \frac{p^2}{2m} + \sum_{i=1}^{N}\left(\frac{p_i^2}{2M} + V(x - R_i)\right). \tag{19}$$

This is similar to an atom consisting of N electrons which have no interaction among themselves but only with the nucleus (which in our case is the single fermion). Transforming to the centre-of-mass (which is *not* the 'nucleus') and to coordinates relative to the 'nucleus' one obtains [14, 15]

$$\hat{H}_{N+1} = \frac{P^2}{2(NM+m)} + \sum_{i=1}^{N}\left(\frac{p_i^2}{2\mu} + V(r_i)\right) + \sum_{i\neq j}\frac{p_i \cdot p_j}{2m}. \tag{20}$$

The last term—the so-called Eckart term—is a genuine two-body interaction and is responsible for the coupling among the particles. Otherwise, the ground-state energy E_N would be just the sum of single-particle energies ϵ_0 and the quantity

$$\Omega \equiv E_{\text{trial}} + \lim_{\beta\to\infty}\frac{1}{\beta}\langle S_0 - S_{\text{trial}}\rangle_{S_{\text{trial}}} = \epsilon_0 - \frac{\partial}{\partial N}E_N\bigg|_{N=1} = -\frac{\partial}{\partial N}\frac{E_N}{N}\bigg|_{N=1} \tag{21}$$

would vanish identically. In the following, Ω will be called the 'kinetic' term as it is the part of the variational bound for the ground-state energy

$$E_0 \leqslant \Omega + \langle S_1\rangle_{S_{\text{trial}}} \tag{22}$$

which does not depend explicitly on the coupling constant α. It is precisely this insufficient bound for Ω which makes the more general approach of LL inferior compared with Feynman's. By using the replica trick, the problem has now been transformed into determining the *chemical potential* $\mu = \partial E_N/\partial N$ at $N = 1$ with the Hamiltonian (20). Equivalently, from equation (21), one has to determine the energy per particle beyond the Hartree approximation, i.e. the correlation energy of the system. Of course, for the harmonic interaction (8), this can be determined exactly by finding the normal modes [16]. The result is

$$E_N^{\text{harmonic}} = \tfrac{3}{2}w(N-1) + \tfrac{3}{2}w\sqrt{NM+m}. \tag{23}$$

Using equation (8*a*), it is easily confirmed that this leads to the correct Feynman result

$$\Omega^{\text{harmonic}} = \frac{3}{4v}(v-w)^2. \tag{24}$$

For a general potential and for small coupling constants, the kinetic term Ω can be calculated systematically by considering the Eckart term as a perturbation. This is possible

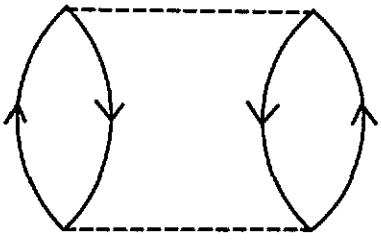

Figure 1. Second-order Goldstone diagram for the kinetic term Ω with the Eckart term as a two-body interaction. The rules are the same as for the evaluation of the ground-state energy [17] except for an additional factor $-(n_\ell - 1)$ where n_ℓ is the number of loops.

because, practically, the 'nucleus' does not move in this limit ($m \gg M$). The simplest way of dealing with N bosons (which can condense) is to treat them as fermions and to assign an internal 'spin' to them with N magnetic components [13]. Each loop in a Goldstone diagram for the ground-state energy then carries a factor N. The particular separable form of the Eckart term, as a two-body interaction, leads to considerable simplifications: only an even number of interactions on any particle or hole line is possible due to parity conservation. In addition, one-loop diagrams can be dismissed for the perturbative evaluation of Ω since linear terms in N do not contribute to equation (21).

It has already been noted that the Hartree term gives a zero contribution to Ω. There are no first-order Goldstone diagrams. In second order, the only diagram which survives is the one shown in figure 1 and its contribution is given by

$$\Omega^{(2)} = \frac{1}{2m^2} \sum_{a,b} \frac{|p_{0a} \cdot p_{0b}|^2}{\epsilon_a + \epsilon_b - 2\epsilon_0} \tag{25}$$

where $p_{0a} = \langle 0|p|a\rangle$ is the single-particle matrix element of the momentum operator in the basis of eigenstates of $\hat{H}_2$. In third order, one finds that from the fourteen Goldstone diagrams for the energy [18], only the four shown in figures 2(a)–2(d) contribute with relative weight—2, 1, 1 and 1, respectively. This gives

$$\Omega^{(3)} = \frac{1}{m^3} \sum_{a,b,c} \frac{p_{0b} \cdot p_{0c} p_{c0} \cdot p_{0a} p_{a0} \cdot p_{c0}}{(\epsilon_b + \epsilon_c - 2\epsilon_0)(\epsilon_a + \epsilon_b - 2\epsilon_0)}. \tag{26}$$

As a check, it is useful to evaluate equations (25) and (26) for the harmonic interaction (8). This is very easy because only one excited p-state contributes to each sum. One finds $\Omega^{(2)} = 3(v^2 - w^2)^2/16v^3$ and $\Omega^{(2)} + \Omega^{(3)} = \Omega^{(2)}(1 + (v^2 - w^2)/2v^2)$ which agrees with the exact result up to terms of $\mathcal{O}(\alpha^3)$ and $\mathcal{O}(\alpha^4)$, respectively. The ring diagrams shown in figures 1 and 2 can be summed by diagonalizing the Hamiltonian (20) in a basis made up by the zeroth- and first-order perturbative wavefunction. As shown in appendix A, one obtains

$$\Omega^{\text{ring}} = \frac{\Omega^{(2)}}{1 - \Omega^{(3)}/\Omega^{(2)}} \tag{27}$$

which is somewhat better than the perturbative result for large couplings constants: for a harmonic interaction it gives one half of the exact result compared with 3/8 of the exact result when $\Omega^{(2)}$ and $\Omega^{(2)}$ are added.

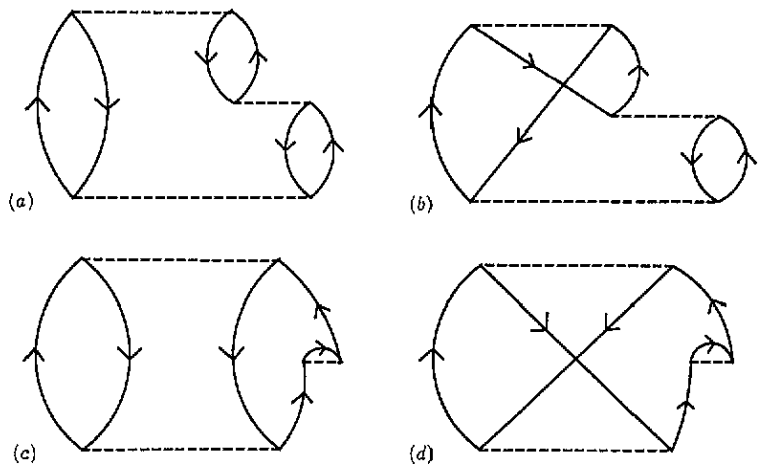

Figure 2. Third-order Goldstone diagrams for Ω.

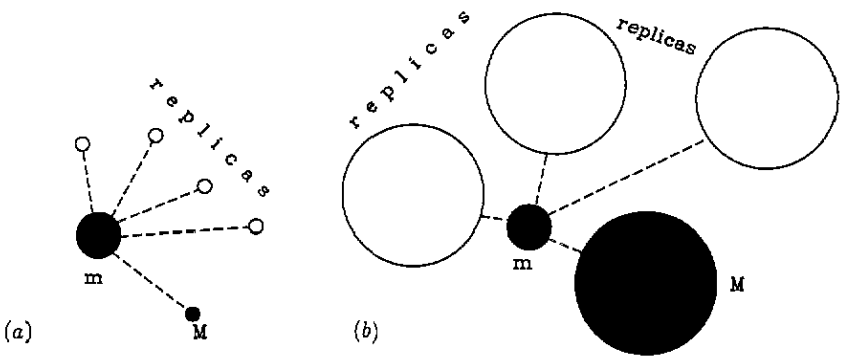

Figure 3. Schematic drawing of the particle–shadow system together with the shadow replicas as described by the Hamiltonian (19). The broken lines represent the potential $V(x - R_i)$ between the particle and the shadows, whereas the size of the circles indicates the corresponding masses: (*a*) small coupling constants where $m \gg M$; (*b*) large coupling constants for which $m \ll M$.

However, the resummation in equation (27) is still insufficient for large coupling constants since it only contains particle–hole interactions and leaves out particle–particle interactions. In this limit the replicas become very massive and do not move much whereas the fermion is now the light particle. This is a situation reminiscent of the treatment of nuclear motion in molecules when the Born–Oppenheimer approximation applies. As is well known [19] the energy of the electrons (the fermion in our case) depends parametrically on the coordinates of the nuclei (the replicas) and serves as a potential for the latter ones. For $M \to \infty$, the ground-state energy is then the minimum of $\epsilon_0(\boldsymbol{R}_1, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N)$ with corrections coming from harmonic vibrations around the minimal points. As the replicas do not interact with each other, these minimal positions are all the same. Taking into account that the difference between m and μ is negligible for large M, it then follows from equation (19) that the ground-state energy of the system is $\epsilon_0^{(2)}[V \to NV]$. Using the Hellmann–Feynman theorem [20, 14] to perform the N-differentiation we therefore obtain from equation (21)

$$\Omega \overset{M\gg m}{\longrightarrow} \epsilon_0 - \langle 0|V|0\rangle = \langle 0|\frac{p^2}{2\mu}|0\rangle \tag{28}$$

i.e. the kinetic term is given by the mean kinetic energy of the particle in the ground state of $\hat{H}_2$. As shown by LL, this leads to the correct Pekar limit for the self-energy at large coupling. However, in the LL approach, equation (28) is used for *all* coupling constants, which is not justified as the role of heavy and light particles reverses at smaller coupling. This is illustrated in figure 3.

4. Variational bounds

Calculating the kinetic term Ω for weak and strong coupling is not very useful for several reasons. First, perturbative calculations can be easily performed for the full field-theoretical problem defined by equation (1) so that a perturbative calculation in an approximate context does not make much sense. In the polaron problem, the same applies for the strong-coupling case. It is exactly this intermediate coupling case where discrepancies exist between Monte Carlo calculations [8] and approximate analytical methods [21]. Second, by evaluating Ω approximately, the variational bound for the self-energy is lost in most cases.

An exception is the resummation (27) of ring diagrams which can be shown to yield a lower bound for Ω (see appendix A). However, what really is needed for the variational principle (22) is an *upper* bound. This can be obtained in several ways. One is by recognizing that $\Omega = \epsilon_0 - \mu$ is the *thermodynamical potential* at zero temperature and mean particle number $N = 1$ for which well known variational bounds exist [22, 23]. I have not succeeded in finding any simple ansätze which lead to any useful results. Another possibility seems to be deriving a lower bound for

$$\frac{\partial}{\partial N} E_N \bigg|_{N=1} = \lim_{N\to 1} \frac{E(N) - E(1)}{N-1}. \tag{29}$$

Since $E(1) = \epsilon_0$ is known exactly this requires a lower bound for the ground-state energy such as Temple's bound [24, 14]

$$E_0 \geqslant \bar{E} - \frac{\langle\psi|(\hat{H}_{N+1} - \bar{E})^2|\psi\rangle}{E_1 - \bar{E}}. \tag{30}$$

Here $\bar{E} = \langle\psi|\hat{H}_{N+1}|\psi\rangle$ and E_1 denotes the exact first-excited-state energy of the $(N+1)$-particle system. The appearance of the latter quantity, which is difficult to estimate, constitutes a major disadvantage of this approach. In addition, the analytic continuation from integer N to $N \to 1$ in equation (29) may lead to a loss of the variational bound although stationarity still holds.

Instead, it seems to be better to deal directly with the path integral (16). Using the concavity of the logarithmic function (or simply by looking at a plot of $\log x$), the following inequality can be easily derived

$$\log B \leqslant \log B_{\text{trial}} + \frac{B}{B_{\text{trial}}} - 1 \tag{31}$$

which is valid for $B, B_{\text{trial}} > 0$ [26]. Several choices are possible for the trial-functional B_{trial}: one may choose a quadratic form in $x(t)$ which would be exact for harmonic

interactions (cf [27]) but has the disadvantage of being inadequate for strong coupling. Instead, let us take the translationally invariant trial-functional

$$B_{\text{trial}}[\boldsymbol{R}, x] = C \exp\left(- \int_0^\beta \mathrm{d}t\, \tilde{V}(\boldsymbol{R} - x) \right) \tag{32}$$

with a constant C and a potential function $\tilde{V}$ to be varied. It is easily seen that the path integrals which occur if equations (31), (32) are used in equation (16) can be translated into quantum-mechanical expectation values involving the *three-body* Hamiltonian

$$\hat{H}_3 = \frac{\boldsymbol{P}^2}{2(2M+m)} + \frac{\boldsymbol{p}_1^2}{2\mu} + V(\boldsymbol{r}_1) - \tilde{V}(\boldsymbol{r}_1) + \frac{\boldsymbol{p}_2^2}{2\mu} + V(\boldsymbol{r}_2) + \frac{\boldsymbol{p}_1 \cdot \boldsymbol{p}_2}{m}. \tag{33}$$

Varying the constant C gives

$$\Omega[\tilde{V}] \leqslant 2\epsilon_0^{(2)} - \langle 0|\tilde{V}|0\rangle - \epsilon_0^{(3)} \tag{34}$$

where $\epsilon_0^{(3)}$ is the ground-state energy associated with the Hamiltonian $\hat{H}_3$. In deriving equation (34), use has been made of the relation

$$\lim_{\beta\to\infty} \frac{1}{\beta} \int_0^\beta \mathrm{d}t\, \langle \tilde{V}(\boldsymbol{r}(t))\rangle_{S_{\text{trial}}} = \langle 0|\tilde{V}(\boldsymbol{r})|0\rangle \tag{11c}$$

between path-integral averages and ground-state expectation values which, e.g., follows from equation (11*b*). Variation with respect to $\tilde{V}$ shows that for strong coupling $\tilde{V} \to V$. In this case $\epsilon_0^{(3)} \to \epsilon_0^{(2)}$ and therefore one obtains $\Omega \leqslant \epsilon_0 - \langle 0|V|0\rangle$ which is the correct strong-coupling limit (28) and leads to the Pekar limit for the self-energy. For small coupling, however, first-order perturbation theory gives

$$\epsilon_0^{(3)} = 2\epsilon_0 + \langle 00|U|00\rangle + \mathcal{O}(U^2) \tag{35}$$

taking $U \equiv \boldsymbol{p}_1 \cdot \boldsymbol{p}_2/m - \tilde{V}$ as perturbation. This has the consequence that $\tilde{V}$ cancels in equation (34) in first order and, since it only acts on one particle, one obtains in second order

$$\Omega \leqslant \frac{1}{m^2} \sum_{a,b} \frac{|\boldsymbol{p}_{0a} \cdot \boldsymbol{p}_{0b}|^2}{\epsilon_a + \epsilon_b - 2\epsilon_0} + \sum_{n\neq 0} \frac{|\tilde{V}_{0n}|^2}{\epsilon_n - \epsilon_0} + \mathcal{O}(U^3). \tag{36}$$

Obviously the best which can be achieved by varying $\tilde{V}$ is $\tilde{V} = \mathcal{O}(\alpha^2)$ so that it does not contribute to equation (36) in the order considered. Comparing with equation (25) one then sees that the present variational bound only gives $\Omega \leqslant 2\Omega^{(2)}$ at small coupling constants.

Although this is considerably better than LL's result it is unclear *a priori* whether the variational determination of the best potential $V(r)$ compensates for this deficiency at small coupling constants. To answer this question, one has to minimize $\Omega + \langle S_1\rangle_{S_{\text{trial}}}$ with respect to the potential $V(r)$ which up to now was considered to be fixed. In the polaron case, it is well known that for small coupling the ground-state energy has the expansion

$$E_0 = -\alpha - c_2\alpha - \cdots \tag{37}$$

and that the exact result is $c_2 = 0.015\,920$ whereas the Feynman approximation gives $c_2^{\mathrm{F}} = 1/81 = 0.012\,346$. In appendix B, it is shown that in the present approach the best potential is *not* harmonic at small coupling and that the corresponding coefficient is $c_2^{\mathrm{S}} = (1 - 8/(3\pi))/12 = 0.012598$. This is the same result as that obtained by Adamowski *et al* [28] and Saitoh [29] who considered the most general quadratic trial action and it represents only a small improvement over Feynman's result. In addition, appendix B demonstrates that an insufficient kinetic term Ω, such that at small coupling $\Omega \to \lambda\Omega^{(2)}$ with a constant $\lambda \geqslant 1$, translates into $c_2 \to c_2^{\mathrm{S}}/\lambda$. Thus the aforementioned factor of two in the variational three-body bound for Ω still renders the present approach in the polaron case inferior to Feynman's for $\alpha \ll 1$ although it will do better for larger α since it embodies the correct large-coupling limit.

Finally, I would like to mention that, in principle, one could derive better bounds by sharpening the logarithmic inequality (31) to

$$\log x \leqslant \sum_{k=1}^{2l+1} \frac{(-)^{k+1}}{k} (x-1)^k \tag{38}$$

which is valid for $x > 0$. However, this would require solving a quantum-mechanical $(2l+3)$-body problem and thus does not seem practical beyond $l = 0$. Already the three-body bound (34) poses a formidable numerical problem for intermediate coupling constants.

5. Summary

I have given an improved description of an approximate mapping of (non-relativistic) field theory to many-body quantum mechanics following the work of LL. The physical picture associated with this approximation is simple and appealing: the cloud of bosons surrounding the fermion is represented by a 'shadow' particle which interacts with the fermion via an effective potential. Surprisingly enough, it is not the interaction term but the kinetic term in the variational principle which is the challenging part for analytic evaluation of the various averages. The variational bound derived for this term in the present work requires, in general, the solution of a three-body problem with separable two-body interactions. Compared with the exactly solvable case of a harmonic potential it is still inferior to Feynman's ansatz for small coupling constants but eventually becomes better as it has the correct large-coupling limit built in. This can be traced back to the use of an additional inequality for the logarithmic function. As the motivation for the present study was to avoid the double use of Jensen's inequality, which badly affected LL's result this outcome is not fully satisfactory. However, it should be kept in mind that, for small coupling constants, perturbation theory is available and it is at intermediate and large coupling constants where *non-perturbative* methods are badly needed. In these cases, the present variational bounds might yield useful results.

The relevance of such an approach is not only that it is a very successful non-perturbative method in the polaron case. As the particle–shadow interaction is formulated in ordinary quantum mechanics, it may also be expected that spin- and isospin-dependent interactions (as in the pion–nucleon case) can be handled similarly. Due to the fact that spin in a path integral inherently involves complex actions [30, 31], I expect that the variational solutions for the self-energy in this case are only stationary and are no longer upper bounds for the true energy. Finally, I note that such 'shadows' have been introduced phenomenologically in models for the confinement of quarks in quantum chromodynamics [32]. The main

feature there is a non-Hermitean constant effective potential which leads to the eventual decay of free quarks and therefore to their non-observation at asymptotic distances. This may arise from the non-Abelian nature of quantum chromodynamics in contrast to the simple Yukawa-type field theories considered here. Needless to say that questions of gauge invariance, relativistic covariance and renormalization, which have not been considered here at all, have to be answered before progress in this direction can be made.

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Appendix A. Summation of ring diagrams

In order to sum the ring diagrams, I will diagonalize the $(N+1)$-body Hamiltonian

$$H_{N+1} = H_0 + V \tag{A.1}$$

within a space spanned by the orthonormalized states

$$|\Psi_0\rangle = |0,0\ldots0\rangle \qquad \text{and} \qquad |\Psi_1\rangle = C\frac{Q_0}{H_0 - E^{(0)}}V|\Psi_0\rangle. \tag{A.2}$$

Here H_0 is the one-body part of the Hamiltonian, $E^{(0)} = N\epsilon_0$ denotes the energy of the unperturbed Hartree state and $V = \sum_{i<j} p_i \cdot p_j/m$ is the Eckart term. $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are zeroth- and first-order perturbative wavefunctions, respectively, and $Q_0 = 1 - |\Psi_0\rangle\langle\Psi_0|$ denotes the projection operator which excludes the unperturbed ground state.

As usual the ground-state energy of a two-state system is given by

$$E_N = \tfrac{1}{2}(H_{00} + H_{11}) - \tfrac{1}{2}\sqrt{(H_{11} - H_{00})^2 + 4|H_{01}|^2}. \tag{A.3}$$

For the matrix elements one finds

$$H_{00} = E^{(0)} \tag{A.4}$$

$$H_{01} = \frac{E^{(2)}}{\sqrt{E^{(2)'}}} \tag{A.5}$$

$$H_{11} = E^{(0)} + \frac{1}{2E^{(2)'}}(E^{(2)} + E^{(3)}) \tag{A.6}$$

with

$$E^{(2)} = \langle\Psi_0|V\frac{1}{H_0 - E^{(0)}}V|\Psi_0\rangle = N(N-1)\Omega^{(2)} \tag{A.7}$$

$$E^{(2)'} = \langle\Psi_0|V\frac{1}{(H_0 - E^{(0)})^2}V|\Psi_0\rangle = \frac{N(N-1)}{2}\frac{\partial}{\partial\epsilon_0}\Omega^{(2)} \tag{A.8}$$

$$E^{(3)} = \langle\Psi_0|V\frac{1}{H_0 - E^{(0)}}V\frac{1}{H_0 - E^{(0)}}V|\Psi_0\rangle = N(N-1)(N-2)\Omega^{(3)}. \tag{A.9}$$

Only constant and linear terms in $(N-1)$ are needed for the calculation of Ω. By expanding equation (A.3) in powers of $(N-1)$, one obtains

$$E_N = \epsilon_0 + (N-1)\epsilon_0 - (N-1)\frac{\Omega^{(2)2}}{\Omega^{(2)} - \Omega^{(3)}} + \mathcal{O}((N-1)^2) \tag{A.10}$$

from which equation (27) follows. The same result is obtained by a variational calculation with

$$|\Psi\rangle = Z_0|\Psi_0\rangle + Z_1|\Psi_1\rangle \tag{A.11}$$

as a trial function which shows that equation (A.10) is an upper bound for the energy. Consequently, Ω^{ring} is a lower bound for the true kinetic term.

Appendix B. Variational solution for small coupling

In this section, I derive the small-coupling limit of the polaron energy in the present approach. This is achieved by expanding the variational bound (22) for the energy in powers of α, including terms up to order α^2.

We know that $\Omega^{(2)}$, given in equation (25), is correct up to this order. Disentangling the energy denominator by a Laplace transform, it may be written as

$$\Omega^{(2)} = \tfrac{3}{2}\int_0^\infty \mathrm{d}t\, F^2(t) \tag{B.1}$$

where

$$F(t) = \sum_n \exp(-t(\epsilon_n - \epsilon_0))|\langle 0|p_z|n\rangle|^2 = \langle 0|p_z \exp(-t(h-\epsilon_0))p_z|0\rangle \tag{B.2}$$

is the Laplace transform of the single-particle response function associated with the excitation operator p_z. Rotational symmetry of the ground state has been used as well as the usual polaron units ($\omega = m = 1$).

To obtain the small-coupling limit of the interaction term $\langle S_1\rangle_{S_{\text{trial}}}$, it is convenient to use the Fourier-transformed form of equation (15)

$$\langle S_1\rangle_{S_{\text{trial}}} = -\frac{\alpha}{\sqrt{2}\mu}\sum_n \frac{1}{1+\Delta_n}\int \mathrm{d}^3r\,\mathrm{d}^3r'\,\frac{\phi_0(r)\phi_0(r')\phi_n(r)\phi_n(r')}{|r-r'|} \times\left[1-\exp\left(-2C\sqrt{1+\Delta_n}|r-r'|\right)\right] \tag{B.3}$$

where $C = \sqrt{M\mu/2}$ and $\Delta_n = \epsilon_n - \epsilon_0$ (see equation (10) of [10]). At small coupling $M, \mu = \mathcal{O}(\alpha)$ and therefore one can expand the exponential in equation (B.3). However, it must be realized that in this limit the radial extension of the polaron is $\mathcal{O}(\alpha^{-1/2})$ so that one has to expand up to third order. Using orthogonality and completeness of the wavefunctions $\phi_n(r)$ one then obtains

$$\langle S_1\rangle_{S_{\text{trial}}} = -\alpha - \tfrac{1}{2}\alpha M + \tfrac{2}{3}\alpha M^2\gamma + \mathcal{O}(\alpha^3) \tag{B.4}$$

with

$$\gamma = \sum_n \sqrt{1+\Delta_n}|\langle 0|r|n\rangle|^2 - \langle 0|r^2|0\rangle = \langle 0|r\sqrt{1+h-\epsilon_0}r - r^2|0\rangle \geqslant 0. \tag{B.5}$$

The variational energy is a function of the mass M of the shadow particle and a functional of the potential $V(r)$ between electron and shadow. However, the mass parameter also enters into the wavefunctions ϕ_n and the energies ϵ_n. It is convenient to separate this dependence by scaling

$$\xi = \sqrt{M}r \tag{B.6}$$

and defining

$$\bar{V}(\xi) = \lim_{\alpha\to 0} V\left(\frac{r}{\sqrt{M}}\right) \qquad \text{and} \qquad \bar{\epsilon}_n = \lim_{\alpha\to 0}\epsilon_n. \tag{B.7}$$

Then wavefunctions and energies are independent of M

$$\bar{h}\bar{\phi}_n(\xi) \equiv (-\tfrac{1}{2}\Delta_\xi + \bar{V}(\xi))\bar{\phi}_n(\xi) = \bar{\epsilon}_n\phi_n(\xi). \tag{B.8}$$

Similarly, one defines

$$\bar{\Omega} = \lim_{\alpha\to 0}\frac{\Omega^{(2)}}{M^2} \qquad \text{and} \qquad \bar{\gamma} = \tfrac{4}{3}\lim_{\alpha\to 0} M\gamma \tag{B.9}$$

with M-independent (i.e. α-independent) quantities $\bar{\Omega}$ and $\bar{\gamma}$. The variational bound for the ground-state energy now reads

$$E_0[M, V] \leqslant M^2\bar{\Omega} - \alpha - \tfrac{1}{2}\alpha M + \tfrac{1}{2}\alpha M\bar{\gamma} + \mathcal{O}(\alpha^3) \tag{B.10}$$

and the variation with respect to M can be performed easily. The optimal mass parameter is

$$M = \frac{\alpha}{4\bar{\Omega}}(1-\bar{\gamma}) + \mathcal{O}(\alpha^2) \tag{B.11}$$

and the energy has the desired expansion

$$E_0 = -\alpha - c_2\alpha^2 + \mathcal{O}(\alpha^3) \tag{B.12}$$

with

$$c_2 = (1-\bar{\gamma})^2/(16\bar{\Omega}). \tag{B.13}$$

In order for the mass of the shadow particle to be positive, one obviously needs $\bar{\gamma} \leqslant 1$. Note that the coefficient c_2 depends inversely on $\bar{\Omega}$: if, instead of $\Omega^{(2)}$, the small-coupling expansion had been performed with $\lambda\Omega^{(2)}$ where $\lambda \geqslant 1$ then the coefficient c_2 would have been reduced by a factor $1/\lambda$.

The task is now to *maximize* c_2 with respect to the potential $\bar{V}(\xi)$. At first sight this seems impossible to do analytically due to the complicated nonlinear dependence of wavefunctions and energies on $\bar{V}(\xi)$. Still, it is possible if the resulting response function

$\bar{F}(t)$ is varied instead of the potential. This requires that the kinetic term $\bar{\Omega}$ can also be expressed in terms of $\bar{F}(t)$. From equations (B.5) and (B.9), one first derives

$$\tilde{\gamma} = \frac{2}{\sqrt{\pi}} \int_0^\infty \mathrm{d}t \, \frac{\mathrm{e}^{-t}}{t^{3/2}} \left[\bar{G}(0) - \bar{G}(t) \right] \tag{B.14}$$

where

$$\bar{G}(t) = \sum_n \exp(-t(\epsilon_n - \epsilon_0)) |\langle 0|\xi_z|n\rangle|^2 = \langle 0|\xi_z \exp(-t(\bar{h} - \bar{\epsilon}_0))\xi_z|0\rangle \tag{B.15}$$

is the Laplace transform of the response function associated with the (scaled) dipole operator ξ_z. By means of the Heisenberg equations for the dipole operator, one immediately finds $\bar{F}(t) = \bar{G}''(t)$ and, after suitable integrations by parts, one obtains the desired relation

$$\tilde{\gamma} = 1 - 4 \int_0^\infty \mathrm{d}t \left[\left(t + \frac{1}{2} \right) \mathrm{erfc}(\sqrt{t}) - \sqrt{\frac{t}{\pi}} \mathrm{e}^{-t} \right] \bar{F}(t) \equiv 1 - \int_0^\infty \mathrm{d}t \, f(t) \bar{F}(t). \tag{B.16}$$

Here $\mathrm{erfc}(x)$ is the complementary error function. Before performing the variation with respect to the function $\bar{F}(t)$, one should realize that it is not completely arbitrary even for a general local potential: expanding $\bar{G}(t)$ in powers of t one finds

$$\bar{G}(t) = \langle 0|\xi_z^2|0\rangle - t\langle 0|\xi_z(\bar{h} - \bar{\epsilon})\xi_z|0\rangle + \ldots = \langle 0|\xi_z^2|0\rangle - \tfrac{1}{2} t \langle 0|[\xi_z, [\bar{h}, \xi_z]]|0\rangle + \ldots . \tag{B.17}$$

The linear term is identical to the Thomas–Reiche–Kuhn sum rule to which a *local* potential does not contribute. Evaluating the double commutator using equation (B.8), one, therefore, finds

$$-\bar{G}'(0) = \int_0^\infty \mathrm{d}t \, \bar{F}(t) = \tfrac{1}{2} \tag{B.18}$$

as constraint. The variation of c_2 can now be performed: with the ansatz

$$\bar{F}(t) = \frac{w}{2} \mathrm{e}^{-wt} \tag{B.19}$$

one obtains $w^{\max} = 3$ and $c_2^{\max} = 1/81$ which is the small-coupling limit of Feynman's approximation. However, one can do better by varying with respect to the full function $\bar{F}(t)$ under the constraint (B.18). A simple calculation yields

$$\bar{F}(t)^{\max} = \frac{f(t)}{2 \int_0^\infty \mathrm{d}t \, f(t)} \tag{B.20}$$

and

$$c_2^{\max} = \frac{1}{24} \int_0^\infty \mathrm{d}t \, f^2(t) \tag{B.21}$$

with $f(t)$ being defined in equation (B.16). The integrals involving the error function can all be performed analytically by appropriate integrations by parts and one obtains

$$c_2^{\max} = \frac{1}{12} \left(1 - \frac{8}{3\pi} \right).$$

Using equation (B.11), the corresponding mass of the shadow particle is $M = \alpha/6 + \mathcal{O}(\alpha^2)$ which agrees with the small-coupling expansion of the polaron effective mass $m^* \simeq 1 + M$. It is unclear which local potential generates $\bar{F}(t)^{\max}$ in equation (B.20) but it is certainly not harmonic as comparison with equation (B.19) shows.

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