# Exact Ground State Energy of the Strong-Coupling Polaron

Elliott H. Lieb[1] and Lawrence E. Thomas[2]

[1] *Departments of Physics and Mathematics, Jadwin Hall, Princeton University, P. O. Box 708, Princeton, New Jersey 08544*

[2] *Department of Mathematics, University of Virginia, Charlottesville, Virginia 22903*

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**Abstract**

The polaron has been of interest in condensed matter theory and field theory for about half a century, especially its strong coupling limit. It was not until 1983, however, that a proof of the asymptotic formula for the ground state energy was finally given by using difficult arguments involving the large deviation theory of path integrals. Here we derive the same asymptotic result, $E_0 \sim -C\alpha^2$, and with explicit error bounds, by simple, rigorous methods applied directly to the Hamiltonian. Our method is easily generalizable to other settings, e.g., the excitonic and magnetic polarons.

The polaron Hamiltonian of Fröhlich [1] is a model for the Coulomb interaction of one or more electrons with the phonons of an ionic crystal. In the course of time it was also seen to be an interesting field theory model of non-relativistic particles interacting with a scalar boson field, and it was widely studied [2, 3, 4, 5, 6, 7] in both contexts.

The model has one dimensionless coupling constant, $\alpha$, and it was noticed very early that there seems to be a qualitative difference in the ground state between the weak coupling regime, well described by perturbation theory [8], in which the electron is spread out, and the strong coupling regime in which the electron appears to be trapped in a phonon hole of its own making. By now it seems doubtful that such a trapping actually occurs [7, 9, 10], but it remains true that the calculation of the ground state energy, $E_0(\alpha)$, is very different in the two regimes. The strong coupling theory was studied by Pekar [2] (see also [3, 4, 5]) who hypothesized that in this limit the total ground state wave function $\Psi$ could be taken to be a product of an electronic function $\phi(x)$ and a phonon function $|\xi\rangle$.

Fröhlich's Hamiltonian in appropriate units is

$$H = \mathbf{p}^2 + \sum_{\mathbf{k}} a_{\mathbf{k}}^* a_{\mathbf{k}} + (\frac{4\pi\alpha}{V})^{1/2} \sum_{\mathbf{k}} \left[ \frac{a_{\mathbf{k}}^*}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} + h.c. \right] \tag{1}$$

where $\mathbf{p} = -i\nabla$ is the electron momentum operator, $\mathbf{x}$ is its coordinate, and $V$ is the volume of the crystal, which tends to infinity. The $\mathbf{k}$'s are the usual normal modes and, as usual, $V^{-1}\sum_{\mathbf{k}} \to (2\pi)^{-3}\int d^3k$. When $\langle\Psi|H|\Psi\rangle$ is computed with Pekar's ansatz one easily finds that the phonon part $|\xi\rangle$ can be easily evaluated by 'completing the square' and the resulting $\phi$ minimizes the energy

$$\mathcal{E}(\phi) \equiv \int |\nabla\phi|^2 d^3x - \alpha \int\int \frac{\phi(\mathbf{x})^2\phi(\mathbf{y})^2}{|\mathbf{x}-\mathbf{y}|} d^3x d^3y \tag{2}$$

subject to $\int \phi(\mathbf{x})^2 d^3x = 1$.

It has been proved [11] that there is exactly one $\phi$, up to translations, that minimizes $\mathcal{E}(\phi)$. By scaling, the minimum energy (call it $E_P(\alpha)$) is proportional to $-\alpha^2$. The question we address is this: *Is this energy, $E_P(\alpha)$, asymptotically exact as $\alpha$ tends to infinity?* Since it is given by a variational calculation, $E_P(\alpha)$ is an upper bound to $E_0(\alpha)$; the problem is to find a lower bound that agrees with $E_P(\alpha)$ to leading order. For a long time more or less the only thing that could be done to validate $E_P(\alpha)$ was a lower bound [12] of the right order, $-\alpha^2$, but which was about a factor of 3 too large. It was not until 1983, with a precursor in [13], that a complete proof was given [14]. The proof starts with an expression [15] for $E_0$ in terms of a self-interacting Brownian path, obtained from the Feynman-Kac formula for $e^{-\beta H}$ by integrating out the phonon variables. This proof is very far from simple and requires an enormous knowledge of large deviation theory of Brownian motion, a subject unknown to most physicists, and it does not generalize easily to other models.

In any event, there is the following problem: The Pekar ansatz is based on the physically appealing notion that at large coupling the phonons cannot follow the rapidly moving electron (as they do at weak coupling) and so resign themselves to interacting only with the 'mean' electronic density, $\phi(\mathbf{x})^2$. What, exactly, do these somewhat anthropomorphic words mean? If they are so very physical, they should be quantifiable and it should not take four decades to build a proof of their correctness. Moreover, one should be able to find a proof that is relatively simple (since the idea is a simple one), and that yields some kind of quantitative error estimate. It should also be robust enough to allow an easy extension to some variations of $H$, such as having several electrons instead of one (the polaronic exciton), inclusion of magnetic fields, an electron kinetic energy other than $\mathbf{p}^2$, accommodation of $\mathbf{k}$-dependence and nonlinearity in the phonon self energies, electron-phonon interaction energies other than $1/|\mathbf{k}|$, etc.

The method we present here satisfies, we believe, the criteria of simplicity and robustness. For this reason it might be of general interest in condensed matter theory or field theory. Despite its generality we shall, for clarity, restrict our discussion to the original Hamiltonian, $H$. Our bound on the error is $O(\alpha^{9/5})$, to be compared with the main term $O(\alpha^2)$.

Before going into the details, however, it is helpful to give an overview of our method. The first thing to notice is that Pekar's ansatz amounts, mathematically, to saying that we can replace the operators $a_\mathbf{k}$ by c-numbers $\xi_\mathbf{k}$. One might think, at first, that such a replacement always leads to a lower bound for the energy, but this is false. (If it were true, the small $\alpha$ energy would have to be proportional to $-\alpha^2$ instead of the correct value $-\alpha$.) To pursue this idea, nevertheless, the natural tool to use is coherent states for each phonon mode $\mathbf{k}$. As is well known, these states are indexed by complex numbers $\xi = p + iq$ and, if $|\xi\rangle\langle\xi|$ is the projector onto the coherent state $|\xi\rangle$, we have that $\int |\xi\rangle\langle\xi| \; d\xi d\xi^* = I$ and $\int \xi \; |\xi\rangle\langle\xi| \; d\xi d\xi^* = a$ and $\int (|\xi|^2 - 1)|\xi\rangle\langle\xi| \; d\xi d\xi^* = a^* a$. *It is the extra term $-1$ that kills the lower bound and gives an unwanted energy $-1$ for each phonon mode* (and hence a negative contribution to the energy that is infinite both because there is no infrared and no ultraviolet cutoff). In other words, coherent states would give us what we want (effectively replacing the operator $a$ by the number $\xi$), were it not for the unfortunate fact that the positive operator $a^*a$ is represented by the nonpositive function $|\xi|^2 - 1$.

Our remedy will be to reduce the effective number of phonon modes to a *finite* number of $O(\alpha^{9/5})$, independent of $V$. These modes will be quite different from the original $a_\mathbf{k}$ modes; indeed they will be the $a_\mathbf{k}$ modes summed over boxes in $\mathbf{k}$-space of size $\alpha^{3/5}$. Thus, our physical description of strong coupling will be a little different from the conventional one. *Instead of saying that the phonons cannot follow the electron, our point of view will be that the electron significantly excites only finitely many field modes.*

This mode reduction is accomplished in several steps which can be outlined as follows.

• **I.** Using a simple commutator estimate (as in the elementary proof of Heisenberg's uncertainty principle) we can show that $|\mathbf{k}|$ values larger than $K \approx \alpha^{6/5}$ can be ignored with an energy cost of only $\alpha^{9/5}$. This eliminates the ultraviolet problem, i.e., the fact that $\mathbf{k}^{-2}$ is not summable.

• **II.** With the same energy error we can localize the electron to a cube of side length $\alpha^{-9/10}$.

• **III.** We decompose the ball $|\mathbf{k}| < K$ into blocks of size $\alpha^{3/5}$, each containing $n$ $\mathbf{k}$-values (with $n \sim V\alpha^{9/5}$). There are about $\alpha^{9/5}$ blocks. Because the electron coordinate $\mathbf{x}$ has been localized, the function $\exp(i\mathbf{k}\cdot\mathbf{x})$ in $H$ can be replaced, in a block $B$, by $\exp(i\mathbf{k}_B\cdot\mathbf{x})$, where

$\mathbf{k}_B$ is any conveniently chosen point in $B$. The effect of this decoupling is that the electron interacts only with the one mode $A_B \approx n^{-1/2} \sum_{\mathbf{k}\in B} a_{\mathbf{k}}$, from block $B$. Thus, the electron ends up interacting with only $\alpha^{9/5}$ modes.

• **IV.** These active modes can now be represented by coherent state integrals, as above. The unwanted $-1$ term now contributes only $\alpha^{9/5}$ to $E_0$, that being the number of modes.

The details will now be given.

**I.** We first establish a commutator inequality which will show that the large $\mathbf{k}$ modes of the Hamiltonian may be discarded at the price of only a small decrease in the coefficient of the $\mathbf{p}^2$ term of the Hamiltonian. For any normalized state with expectation $\langle\cdot\rangle$, we have

$$\begin{aligned} |k_j|\,|\langle a^*_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\rangle| &= |\langle [p_j, a^*_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}]\rangle| \\ &\leq 2\langle p_j^2\rangle^{1/2}\langle a^*_{\mathbf{k}} a_{\mathbf{k}}\rangle^{1/2} \end{aligned} \tag{3}$$

for each phonon momentum coordinate $k_j$, $j = 1, 2, 3$, just by the Schwarz inequality. Squaring this inequality, summing over $j$, and then taking the square root, we obtain

$$|\langle a^*_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\rangle| \leq \frac{2}{|\mathbf{k}|}\langle \mathbf{p}^2\rangle^{1/2}\langle a^*_{\mathbf{k}} a_{\mathbf{k}}\rangle^{1/2}. \tag{4}$$

A similar inequality holds for $a^*_{\mathbf{k}}$ replaced by $a_{\mathbf{k}}$. It follows that for any $\varepsilon > 0$, and with $K \equiv 8\alpha/\pi\varepsilon$,

$$\begin{aligned} &-(\frac{4\pi\alpha}{V})^{1/2} \sum_{|\mathbf{k}|\geq K} [\langle \frac{a^*_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}}\rangle + c.c.] \\ \leq\ & 4(\frac{4\pi\alpha}{V})^{1/2}\langle \mathbf{p}^2\rangle^{1/2} \sum_{|\mathbf{k}|\geq K} |\mathbf{k}|^{-2}\langle a^*_{\mathbf{k}} a_{\mathbf{k}}\rangle^{1/2} \\ \leq\ & 4(\frac{4\pi\alpha}{V})^{1/2}\langle \mathbf{p}^2\rangle^{1/2}(\sum_{|\mathbf{k}|\geq K} |\mathbf{k}|^{-4})^{1/2}(\sum_{|\mathbf{k}|\geq K}\langle\ a^*_{\mathbf{k}} a_{\mathbf{k}}\rangle)^{1/2} \\ =\ & 2\varepsilon^{1/2}\langle \mathbf{p}^2\rangle^{1/2}(\sum_{|\mathbf{k}|\geq K}\langle\ a^*_{\mathbf{k}} a_{\mathbf{k}}\ \rangle)^{1/2} \\ \leq\ & \varepsilon\langle \mathbf{p}^2\rangle + \sum_{|\mathbf{k}|\geq K}\langle\ a^*_{\mathbf{k}} a_{\mathbf{k}}\ \rangle, \end{aligned} \tag{5}$$

again by the Schwarz inequality. (We have taken the limit $V \to \infty$ in the sum.)

The above inequality (5) is an ultraviolet bound. It shows that the Hamiltonian $H$ is bounded below by a new one $H_K$, i.e., $H \geq H_K$, with

$$H_K \equiv (1 - \frac{8\alpha}{\pi K})\mathbf{p}^2 + \sum_{|\mathbf{k}|<K} a^*_{\mathbf{k}} a_{\mathbf{k}} + (\frac{4\pi\alpha}{V})^{1/2}\left[\frac{a^*_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} + h.c.\right]. \tag{6}$$

By completing the square, we have that

$$a^*_{\mathbf{k}} a_{\mathbf{k}} + (\frac{4\pi\alpha}{V})^{1/2} \left[ \frac{a^*_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} + h.c. \right] \geq -\frac{4\pi\alpha}{|\mathbf{k}|^2 V} \tag{7}$$

and if $K$ is chosen so that the coefficient of $\mathbf{p}^2$ vanishes in $H_K$, i.e., $K = 8\alpha/\pi$, then

$$H \geq H_K \geq -\frac{4\pi\alpha}{V} \sum_{|\mathbf{k}|<K} |\mathbf{k}|^{-2} = -\frac{16}{\pi^2}\alpha^2, \tag{8}$$

showing that $H$ is indeed bounded below by $O(\alpha^2)$. But to obtain the sharp lower bound, we will take a larger $K$, namely $K = (8/\pi c_1)\alpha^{6/5}$. Here and below, the $c_i$'s are constants independent of $\alpha$.

**II.** The next step is to localize the electron. Although a-priori the electron is in the box of volume V, it actually can be confined to a box of much smaller size, with only a slight relative increase in its energy. More precisely, we have the following: Let $\Psi$ be any normalized state of the electron and phonons and define $E \equiv \langle\Psi|H_K|\Psi\rangle$. Then, given $\Delta E > 0$, there exists a function $\phi$ of the electron coordinate $\mathbf{x}$ alone (but depending on $\Psi$), with support in a cube of side length $L = \pi(3/\Delta E)^{1/2}$ such that

$$\langle\phi\Psi|H_K|\phi\Psi\rangle \Big/ \langle\phi\Psi|\phi\Psi\rangle \leq E + \Delta E. \tag{9}$$

To see this, let $\phi(\mathbf{x}) = \prod_{j=1}^3 \cos((\Delta E/3)^{1/2} x_j)$ inside the cube of side length $\pi(3/\Delta E)^{1/2}$ centered at the origin and $\phi = 0$ outside the cube. Let $\phi_{\mathbf{y}}(\mathbf{x}) = \phi(\mathbf{x} - \mathbf{y})$ and consider the integral

$$\begin{aligned} \int \Big( & \langle\phi_{\mathbf{y}}\Psi|H_K|\phi_{\mathbf{y}}\Psi\rangle - (E + \Delta E)\langle\phi_{\mathbf{y}}\Psi|\phi_{\mathbf{y}}\Psi\rangle\Big) d^3y \\ &= \int (|\nabla\phi|^2 - \Delta E|\phi|^2)\, d^3y = 0. \end{aligned} \tag{10}$$

Evidently, there must be a point $\mathbf{y}$ such that at this point, the integrand on the left side of (10) is non-positive (and where $\langle\phi_{\mathbf{y}}\Psi|\phi_{\mathbf{y}}\Psi\rangle$ is non-zero). This $\phi_{\mathbf{y}}$ is the $\phi$ that we need. The electron localization is now complete.

For our purposes, we take $\Delta E = c_2\alpha^{9/5}$, and the assertion above together with the ultraviolet bound then implies that the ground state energy $E_0$ of $H$ satisfies

$$E_0 \geq \inf_{\Psi}{}' \langle\Psi|H_K|\Psi\rangle - c_2\alpha^{9/5} \tag{11}$$

where the infimum is taken over all normalized $\Psi$'s but having their $\mathbf{x}$-support in a cube of side length no larger than $L = (3/c_2)^{1/2}\pi\alpha^{-9/10}$ somewhere in the large volume $V$.

**III.** The next step is to group the phonon modes together into blocks, which we take to be cubes with sides of length $P = c_3\alpha^{3/5}$ or, more precisely, the portion of those cubes lying in the big ball $\{\mathbf{k} : |\mathbf{k}| < K\}$. Let $B$ be a block (cube) of momenta with sides of length $P = c_3\alpha^{3/5}$ and let $\mathbf{k}_B$ be *any point* within this block whose precise position will be determined later. It is clear that the set of momenta $\{\mathbf{k} : |\mathbf{k}| < K\}$ can be covered by $N \equiv \frac{4}{3}\pi K^3/P^3 + \textit{lower order} = (2^{11}/(3\pi^2 c_1^3 c_3^3))\alpha^{9/5} + \textit{lower order}$ such blocks.

Assume that $\mathbf{x}$ itself varies over a cube of side length no bigger than $L$ with center at a point $\mathbf{x}_0$ which we take to be the origin $\mathbf{0}$. (If $\mathbf{x}_0$ is not the origin, phase factors $\exp(\pm i(\mathbf{k}-\mathbf{k}_B)\cdot\mathbf{x}_0)$ standing before $a_{\mathbf{k}}^*$ and $a_{\mathbf{k}}$ in the Hamiltonian $H_K$ are readily eliminated by a unitary transformation involving the phonon variables only.) We have that for $\mathbf{k} \in B$,

$$|e^{i\mathbf{k}\cdot\mathbf{x}} - e^{i\mathbf{k}_B\cdot\mathbf{x}}| \le |(\mathbf{k}-\mathbf{k}_B)\cdot\mathbf{x}| \le \frac{3\pi c_3}{2}(\frac{3}{c_2})^{1/2}\alpha^{-3/10}. \tag{12}$$

Then, for any $\delta > 0$, we have the inequality

$$\begin{aligned}\sum_B \sum_{\mathbf{k}\in B} &\left[\delta a_{\mathbf{k}}^* a_{\mathbf{k}} + (\frac{4\pi\alpha}{V})^{1/2}[\frac{a_{\mathbf{k}}^*}{|\mathbf{k}|}(e^{i\mathbf{k}\cdot\mathbf{x}} - e^{i\mathbf{k}_B\cdot\mathbf{x}}) + h.c.]\right] \\ &\ge -\frac{4\pi\alpha}{\delta V}(\frac{3\pi c_3}{2}(\frac{3}{c_2})^{1/2}\alpha^{-3/10})^2 \sum_{|\mathbf{k}|<K} |\mathbf{k}|^{-2} \\ &= -\frac{108 c_3^2}{c_1 c_2 \delta}\alpha^{8/5},\end{aligned} \tag{13}$$

as in (7). We make the choice $\delta = c_4\alpha^{-1/5}$.

The above inequality (13) permits us to bound $H_K$ (still restricted to states with $\mathbf{x}$-support in a cube of sides with size $L$) from below in the following way:

$$\begin{aligned}H_K \ge (1 \;-\; & c_1\alpha^{-1/5})\mathbf{p}^2 + \sum_B \sum_{\mathbf{k}\in B}\Big[(1 - c_4\alpha^{-1/5})a_{\mathbf{k}}^* a_{\mathbf{k}} \\ + \;\; & (\frac{4\pi\alpha}{V})^{1/2}(\frac{a_{\mathbf{k}}^*}{|\mathbf{k}|}e^{i\mathbf{k}_B\cdot\mathbf{x}} + h.c.)\Big] - \frac{108 c_3^2}{c_1 c_2 c_4}\alpha^{9/5}.\end{aligned} \tag{14}$$

Note that, within a single block, the $a_{\mathbf{k}}^*$- and $a_{\mathbf{k}}$-terms have a common exponential factor. For each block $B$ define a block annihilation operator

$$A_B \equiv (\sum_{\mathbf{k}\in B} |\mathbf{k}|^{-2})^{-1/2} \sum_{\mathbf{k}\in B} \frac{a_{\mathbf{k}}}{|\mathbf{k}|} \tag{15}$$

and its corresponding adjoint $A_B^*$. Then $\sum_{\mathbf{k}\in B} a_{\mathbf{k}}^* a_{\mathbf{k}} \geq A_B^* A_B$ and so the operator terms on the right hand side of (14) exceed the operator $H_K^{block} \equiv H_K^{block}(\{\mathbf{k}_B\})$ defined

$$H_K^{block} \equiv (1 - c_1\alpha^{-1/5})\mathbf{p}^2 + \sum_B \Big[(1-c_4\alpha^{-1/5})A_B^* A_B + (\frac{4\pi\alpha}{V}\sum_{\mathbf{k}\in B}|\mathbf{k}|^{-2})^{1/2}(A_B^* e^{i\mathbf{k}_B\cdot\mathbf{x}} + h.c.)\Big]. \tag{16}$$

Referring to (11) and (14), we can summarize the situation: The ground state energy $E_0$ of $H$ satisfies

$$E_0 \geq \inf_{\Psi} \sup_{\{\mathbf{k}_B\}} \langle\Psi|H_K^{block}|\Psi\rangle - (c_2 + \frac{108c_3^2}{c_1c_2c_4})\alpha^{9/5} \tag{17}$$

where the infimum can now even be taken over $\Psi$'s with no restriction on their $\mathbf{x}$-support, and with the $\mathbf{k}_B$'s chosen optimally, depending on $\Psi$.

**IV.** In order to get a lower bound on $H_K^{block}$, we use the technology of coherent states. Let $|\xi\rangle = \pi^{-1/2}\exp(-\frac{1}{2}|\xi|^2 + \xi A^*)|0\rangle$ denote a normalized coherent state for a single harmonic oscillator. In terms of these states one has the identity

$$\exp(\mu A)\exp(\nu A^*) = \int e^{\mu\xi+\nu^*\xi^*}|\xi\rangle\langle\xi|d\,\xi d\,\xi^*, \tag{18}$$

from which the identities for the operators $a$ and $a^*a$ mentioned in the introduction are readily obtained.

Let $\Psi$ be any normalized state and let $|\xi\rangle = \prod_B|\xi_B\rangle$ denote a tensor product of coherent states of the block modes corresponding to the operators $\{A_B\}$. Set $\Psi_\xi(\mathbf{x}) = \langle\Psi|\xi\rangle_{phonon}$, where the inner product, $\langle\ ,\rangle_{phonon}$, is just over the phonon variables, not $\mathbf{x}$. Then

$$\langle\Psi|H_K^{block}|\Psi\rangle = \int\langle\Psi_\xi|h_\xi|\Psi_\xi\rangle_e \Pi_B d\,\xi_B d\,\xi_B^*, \tag{19}$$

where the inner product in the integrand, $\langle\ ,\rangle_e$, is over the electronic coordinates $\mathbf{x}$, and $h_\xi$ is the Schrödinger operator

$$h_\xi \equiv (1-c_1\alpha^{-1/5})\mathbf{p}^2 + \sum_B \Big[(1-c_4\alpha^{-1/5})(|\xi_B|^2 - 1) + (\frac{4\pi\alpha}{V}\sum_{\mathbf{k}\in B}|\mathbf{k}|^{-2})^{1/2}(\xi_B^* e^{i\mathbf{k}_B\cdot\mathbf{x}} + c.c.)\Big]. \tag{20}$$

Now the supremum over $\mathbf{k}_B$ of (19) exceeds

$$\sup_{\{\mathbf{k}_B\}} \int \Big[(1-c_1\alpha^{-1/5})\langle\Psi_\xi|\mathbf{p}^2|\Psi_\xi\rangle_e - \frac{4\pi\alpha}{(1-c_4\alpha^{-1/5})V}\sum_B\sum_{\mathbf{k}\in B}\frac{|\hat\rho_\xi(\mathbf{k}_B)|^2}{|\mathbf{k}|^2\hat\rho_\xi(\mathbf{0})}\Big]\Pi_B d\xi_B d\xi_B^* - N \tag{21}$$

by completing the square, and where $\hat{\rho}_\xi(\mathbf{k})= \langle\Psi_\xi|\exp(i\mathbf{k}\cdot\mathbf{x})|\Psi_\xi\rangle_e$ is the Fourier transform of $|\Psi_\xi|^2(\mathbf{x})$. (Here, we can remove the $|\mathbf{k}|<K$ restriction on the $\mathbf{k}$-sum.) We emphasize again that were it not for the grouping of the phonons into blocks, then this coherent state estimate would contain a negative constant equal to the number of phonon modes with $|\mathbf{k}|<K$ i.e. a number at least $O(\alpha^2)$ (even if $K$ were chosen optimally), instead of $N=O(\alpha^{9/5})$.

At this point we choose $\mathbf{k}_B$ to be a point in $B$ where the function of $\mathbf{k}$,

$$\int \frac{|\hat{\rho}_\xi(\mathbf{k})|^2}{\hat{\rho}_\xi(\mathbf{0})}\Pi_B d\xi_B d\xi_B^*, \tag{22}$$

is minimal. With this choice, (21) is, in turn, larger than

$$\int \Big[(1-c_1\alpha^{-1/5})\langle\Psi_\xi|\mathbf{p}^2|\Psi_\xi\rangle_e - \frac{4\pi\alpha}{(1-c_4\alpha^{-1/5})V}\sum_{\mathbf{k}}\frac{|\hat{\rho}_\xi(\mathbf{k})|^2}{|\mathbf{k}|^2\hat{\rho}_\xi(\mathbf{0})}\Big]\Pi_B d\xi_B d\xi_B^* - N. \tag{23}$$

But the integrand of this integral is $\langle\Psi_\xi|\Psi_\xi\rangle_e \times \mathcal{E}(\Psi_\xi/(\langle\Psi_\xi|\Psi_\xi\rangle_e^{1/2}))$ , where $\mathcal{E}(\cdot)$ is just the Pekar functional (2), (but with coefficients altered by $O(\alpha^{-1/5})$); the $\mathbf{k}$-sum is the Fourier series for the Coulomb self-energy term of $\mathcal{E}$. Thus, the integral (23) exceeds $(1-c_1\alpha^{-1/5})^{-1}(1-c_4\alpha^{-1/5})^{-2}E_P(\alpha)$, with $E_P(\alpha)$ being the Pekar minimum energy of (2).

Taking into account the altered coefficients in the Pekar functional, the lower bound (17), and the definition of $N$, we obtain

$$E_0(\alpha) \geq E_P(\alpha) - (c_2 + \frac{108c_3^2}{c_1c_2c_4} + \frac{2^{11}}{3\pi^2c_1^3c_3^3} + c_5)\alpha^{9/5} - o(\alpha^{-9/5}) \tag{24}$$

where $E_P(\alpha) = -c_P\alpha^2$, $c_P = 0.109$,[9], and where $c_5 = (c_1+2c_4)c_P$ accounts for the altered coefficients in the variational principle. This completes the proof of the lower bound. Optimizing the coefficients, we find that the $\alpha^{9/5}$-error term in (24) is no greater than $3.822\alpha^{9/5}$.

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