Translation invariance and localized states*

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The method originally suggested by Peierls and Yoccoz for treating localized states as approximate eigenstates of translation-invariant Hamiltonians is discussed in a general way. For many-body systems interacting via two-body potentials, it is shown that the effective mass is correctly given by the method. The translationally best localized state is shown to give the exact energy in the two-body problem. Finally, it is shown that both the strong-coupling and weak-coupling regimes of the polaron can be discussed easily in terms of localized coherent states.

I. INTRODUCTION

In several areas of physics, the Hamiltonian of interest is invariant under translation, but the approximate state vectors commonly used as trial vectors are not eigenvectors of the total momentum operator. Rather, the state vectors are localized around some point in space, usually taken at the origin of coordinates. After the parameters or functions in the state vector have been determined by using the variational principle, it is necessary to attempt to correct for the over-all motion of the system.

Peierls and Yoccoz[1] suggested a natural way of using the set of localized states $|\vec{x}\rangle$ at all points $\vec{x}$ to make this correction. The method seems not to have been widely applied.

In this paper, the suggestion made in Ref. 1 is developed first in an abstract way, so as to emphasize the general connection between localized states and translation invariance. The essential requirement is that states at different points be related by

$$|\vec{x}\rangle = e^{-i\vec{P}\cdot(\vec{x}-\vec{y})}|\vec{y}\rangle\,, \tag{1.1}$$

where $\vec{P}$ is the momentum operator of the system. Translation invariance of H means that

$$[H,\vec{P}\,]=0. \tag{1.2}$$

The general technique for utilizing translation invariance to obtain better approximate eigenstates of H is given in Sec. II.

The techniques of Sec. II are then applied to specific cases. For the shell model

$$H=\int \psi^\dagger(\vec{r})\left(-\frac{\nabla^2}{2M}\right)\psi(\vec{r})d\vec{r} + \tfrac{1}{2}\int \psi^\dagger(\vec{r})\psi^\dagger(\vec{s})V(\vec{r}-\vec{s})\psi(\vec{s})\psi(\vec{r})d\vec{r}\,d\vec{s}, \tag{1.3}$$
$$\vec{P}=-i\int \psi^\dagger(\vec{r})\vec{\nabla}\psi(\vec{r})d\vec{r}\,,$$

where $\psi(\vec{r})$ is a fermion field operator. (It should be noted that in this case the use of field operators is only a convenience that simplifies the notation.) A shell-model state located at $\vec{x}$ is given by

$$|\vec{x};S\rangle=\prod_{i\in S} a^\dagger_{i\vec{x}}|\Omega\rangle\,,$$
$$\psi(\vec{r})|\Omega\rangle=0,\quad \text{all } \vec{r} \tag{1.4}$$
$$a^\dagger_{i\vec{x}}=\int \psi^\dagger(\vec{r})f_i(\vec{r}-\vec{x})d\vec{r}\,.$$

Here S is a set of A integers i, and the f_i are a set of functions, usually chosen orthonormal. The operator $a^\dagger_{i\vec{x}}$ creates a particle in the orbital with wave function f_i centered at $\vec{x}$. The fact that

$$[\psi(\vec{r}),\vec{P}\,]=-i\vec{\nabla}\psi(\vec{r}) \tag{1.5}$$

guarantees that (1.1) is satisfied by the states of the form (1.4). The shell model for two nonidentical particles is discussed in Sec. III, for A particles in Sec. IV. This application is the one to which the suggestion in Ref. 1 was directed. Section IV elaborates on the suggestion in Ref. 1 and corrects the erroneous effective mass calculation given there.

The other example considered is the polaron,[2] where

$$H=\int \psi^\dagger(\vec{r})(-\tfrac{1}{2}\nabla^2)\psi(\vec{r})d\vec{r}+\int a^\dagger(\vec{p})a(\vec{p})d\vec{p} - \frac{\sqrt{\gamma}}{2\pi}\int \frac{e^{i\vec{p}\cdot\vec{r}}}{p}\psi^\dagger(\vec{r})\psi(\vec{r})[a(\vec{p})+a^\dagger(-\vec{p})]d\vec{p}\,d\vec{r}, \tag{1.6}$$
$$\vec{P}=-i\int \psi^\dagger(\vec{r})\vec{\nabla}\psi(\vec{r})d\vec{r}+\int \vec{p}\,a^\dagger(\vec{p})a(\vec{p})d\vec{p}\,,$$
$$\gamma=\alpha\sqrt{2}\,.$$

Here α is the usual coupling constant, H is in units of ω, the phonon frequency, and length and momentum are in units M^{-1} and M, respectively,

where

$$M^2 = m\omega , \tag{1.7}$$

with m the electron mass. In the case of the polaron, only one-ψ-particle states are of interest here. The technique for constructing states $|\vec{x}\rangle$ that satisfy (1.1) is given in Sec. V, where the usual weak-coupling and strong-coupling approximations are discussed in terms of localized coherent states. The polaron is used as an example to show the application of localized-state methods in quantum field theory.

II. TRANSLATION AND LOCALIZED STATES

Suppose that a localized state $|\vec{x}\rangle$ is given. Then an upper bound for the energy is the localized-state (LS) value

$$F_{\mathrm{LS}} = \langle \vec{x} | H | \vec{x} \rangle / \langle \vec{x} | \vec{x} \rangle , \tag{2.1}$$

if F_{LS} is a meaningful expression (it will be seen that there are cases in which it is not meaningful). If the state $|\vec{x}\rangle$ satisfies Eq. (1.1), then it follows immediately from the translation invariance of H that

$$F_{\mathrm{LS}} = \langle \vec{0} | H | \vec{0} \rangle / \langle \vec{0} | \vec{0} \rangle . \tag{2.2}$$

A better value for the energy can be obtained by noting that

$$\begin{aligned} \langle \vec{x} | \vec{y} \rangle &= D(\vec{x} - \vec{y}) , \\ \langle \vec{x} | H | \vec{y} \rangle &= A(\vec{x} - \vec{y}) , \end{aligned} \tag{2.3}$$

where the dependence on the single variable is a consequence of Eqs. (1.1) and (1.2). [Note that

$$F_{\mathrm{LS}} = A(\vec{0})/D(\vec{0}) .] \tag{2.4}$$

Now let

$$|\vec{K}\rangle = (2\pi)^{-3/2} \int e^{i\vec{K}\cdot\vec{x}} |\vec{x}\rangle d\vec{x} ; \tag{2.5}$$

it follows immediately from Eqs. (2.3) that

$$\begin{aligned} \langle \vec{K} | \vec{Q} \rangle &= N(\vec{K}) \delta(\vec{K} - \vec{Q}) , \\ \langle \vec{K} | H | \vec{Q} \rangle &= H(\vec{K}) \delta(\vec{K} - \vec{Q}) , \\ N(\vec{K}) &= \int e^{-i\vec{K}\cdot\vec{x}} D(\vec{x}) d\vec{x} , \\ H(\vec{K}) &= \int e^{-i\vec{K}\cdot\vec{x}} A(\vec{x}) d\vec{x} , \end{aligned} \tag{2.6}$$

so that an approximation for the energy that uses these translated localized states (TLS) is given by

$$F_{\mathrm{TLS}} = \min_{\vec{K}} [H(\vec{K})/N(\vec{K})] . \tag{2.7}$$

For all cases to be considered here, the minimum occurs at $\vec{K} = 0$ and Eq. (2.7) will be used in the form

$$\begin{aligned} F_{\mathrm{TLS}} &= H(\vec{0})/N(\vec{0}) \\ &= \int A(\vec{x}) d\vec{x} \Big/ \int D(\vec{x}) d\vec{x} . \end{aligned} \tag{2.8}$$

Now suppose that the state $|\vec{x}\rangle$ depends on some functions f_i (or parameters c_i; the case of parameters is a simple restriction of the following). Than D, A, and, hence, N, H, F_{LS}, and F_{TLS} are functionals of the f_i. If F_{LS} is meaningful, the simplest approximation to the energy is the localized-state energy E_{LS},

$$\begin{aligned} E_{\mathrm{LS}} &= \min_{f_i} F_{\mathrm{LS}}\{f_i\} \\ &= F_{\mathrm{LS}}\{f_i^{\mathrm{LS}}\} . \end{aligned} \tag{2.9}$$

If the functions f_i^{LS} are determined by solving Eqs. (2.9), then Eq. (2.8) gives a translationally improved localized-state energy E_{TILS},

$$E_{\mathrm{TILS}} = F_{\mathrm{TLS}}\{f_i^{\mathrm{LS}}\} . \tag{2.10}$$

Finally the translationally best localized-state energy E_{TBLS} is

$$\begin{aligned} E_{\mathrm{TBLS}} &= \min_{f_i} F_{\mathrm{TLS}}\{f_i\} \\ &= F_{\mathrm{TLS}}\{f_i^{\mathrm{TBLS}}\} . \end{aligned} \tag{2.11}$$

In view of Eq. (2.10), which can be written

$$E_{\mathrm{TILS}} = \frac{H\{\vec{K}=0, f_i^{\mathrm{LS}}\}}{N\{\vec{K}=0, f_i^{\mathrm{LS}}\}} , \tag{2.12}$$

it is tempting to use as an approximation for the effective mass M^*

$$\frac{1}{2M_a^*} = \lim_{K\to 0} \left[\frac{1}{K^2} \left(\frac{H\{\vec{K}, f_i^{\mathrm{LS}}\}}{N\{\vec{K}, f_i^{\mathrm{LS}}\}} - \frac{H\{0, f_i^{\mathrm{LS}}\}}{N\{0, f_i^{\mathrm{LS}}\}} \right) \right] , \tag{2.13}$$

and this is what was done in Ref. 1. However, this must give too small a value for M^*. For $\vec{K} = 0$, f_i^{LS} actually minimizes $\langle H \rangle$ for states with $\langle \vec{P} \rangle = 0$ (within a particular subspace). For $\vec{K} \neq 0$, the corresponding minimization has not been done yet, so that $\langle H \rangle$ will be too large, M_a^* will be too small.

The remedy is clearly to use a Lagrange multiplier $\vec{v}$ and consider

$$G(\vec{v}) = H - \vec{v}\cdot\vec{P} , \tag{2.14}$$

where $\vec{P}$ is the momentum operator. For fixed $\vec{v}$,

$$F_{\mathrm{LS}}(\vec{v}) = \langle \vec{x} | G(\vec{v}) | \vec{x} \rangle / \langle \vec{x} | \vec{x} \rangle \tag{2.15}$$

gives an approximation for $\langle G(\vec{v}) \rangle$ with momentum expectation

$$\vec{Q}_{\mathrm{LS}} = \langle \vec{x} | \vec{P} | \vec{x} \rangle / \langle \vec{x} | \vec{x} \rangle . \tag{2.16}$$

Similarly, with

$$\begin{aligned} B(\vec{x}, \vec{v}) &= \langle \vec{x} | G(\vec{v}) | \vec{0} \rangle , \\ \vec{C}(\vec{x}) &= \langle \vec{x} | \vec{P} | \vec{0} \rangle , \end{aligned} \tag{2.17}$$

it follows as in Eqs. (2.5) and (2.6) that

$$\begin{aligned}
&\langle \vec{K} \,|\, G(\vec{v}) \,|\, \vec{Q} \rangle = G(\vec{K},\vec{v})\delta(\vec{K}-\vec{Q}),\\
&\langle \vec{K} \,|\, \vec{P} \,|\, \vec{Q} \rangle = \vec{Q}(\vec{K})\delta(\vec{K}-\vec{Q}),\\
&G(\vec{K},\vec{v}) = \int e^{-i\vec{K}\cdot\vec{x}} B(\vec{x},\vec{v})\,d\vec{x},\\
&Q(\vec{K}) = \int e^{-i\vec{K}\cdot\vec{x}} \vec{C}(\vec{x})\,d\vec{x},
\end{aligned} \tag{2.18}$$

so that

$$\begin{aligned}
F_{\mathrm{TLS}}(\vec{v}) &= \min_{\vec{K}}[G(\vec{K},\vec{v})/N(\vec{K})]\\
&= G(\vec{K}_{\vec{v}},\vec{v})/N(\vec{K}_{\vec{v}}),\\
\vec{Q}_{\mathrm{TLS}}(\vec{v}) &= \vec{Q}(\vec{K}_{\vec{v}})/N(\vec{K}_{\vec{v}}).
\end{aligned} \tag{2.19}$$

When $|\vec{x}\rangle$ depends on functions f_i, then the $f_i^{\mathrm{LS},\vec{v}}$ and $f_i^{\mathrm{TLS},\vec{v}}$ depend on $\vec{v}$. Thus E_{LS} depends on $\vec{v}$,

$$\begin{aligned}
&E_{\mathrm{LS}}(\vec{v}) = F_{\mathrm{LS}}\{f_i^{\mathrm{LS},\vec{v}},\vec{v}\} + \vec{v}\cdot\vec{P}_{\mathrm{LS}}(\vec{v}),\\
&\vec{P}_{\mathrm{LS}}(\vec{v}) = \vec{Q}_{\mathrm{LS}}\{f_i^{\mathrm{LS},\vec{v}}\}.
\end{aligned} \tag{2.20}$$

Elimination of $\vec{v}$ gives $E_{\mathrm{LS}}(\vec{P}_{\mathrm{LS}})$ and, hence, M^*_{LS}. The quantities M^*_{TILS} and M^*_{TBLS} are obtained similarly.

III. TWO NONIDENTICAL PARTICLES

For two nonidentical particles, the Hamiltonian is slightly different from Eq. (1.3):

$$H = \int \psi_1^\dagger(\vec{r})\left(-\frac{\vec{\nabla}^2}{2M_1}\right)\psi_1(\vec{r})\,d\vec{r} + \int \psi_2^\dagger(\vec{r})\left(-\frac{\nabla^2}{2M_2}\right)\psi_2(\vec{r})\,d\vec{r} + \int \psi_1^\dagger(\vec{r})\psi_2^\dagger(\vec{s})V(\vec{r}-\vec{s})\psi_2(\vec{s})\psi_1(\vec{r})\,d\vec{r}\,d\vec{s}\,. \tag{3.1}$$

The localized state centered at x is taken to be

$$|\vec{x};f,g\rangle = \int \psi_1^\dagger(\vec{r})f(\vec{r}-\vec{x})\,d\vec{r}\int \psi_2^\dagger(\vec{s})g(\vec{s}-\vec{x})\,d\vec{s}\,|\,\Omega\rangle\,. \tag{3.2}$$

Then

$$\begin{aligned}
D(\vec{x};f,g) &= \int f^*(\vec{r}-\vec{x})f(\vec{r})\,d\vec{r}\int g^*(\vec{s}-\vec{x})g(\vec{s})\,d\vec{s}\,,\\
A(\vec{x};f,g) &= \int f^*(\vec{r}-\vec{x})\left(-\frac{\vec{\nabla}^2}{2M_1}\right)f(\vec{r})\,d\vec{r}\int g^*(\vec{s}-\vec{x})g(\vec{s})\,d\vec{s}\\
&\quad + \int f^*(\vec{r}-\vec{x})f(\vec{r})\,d\vec{r}\int g^*(\vec{s}-\vec{x})\left(-\frac{\vec{\nabla}^2}{2M_1}\right)g(\vec{s})\,d\vec{s} + \int f^*(\vec{r}-\vec{x})g^*(\vec{s}-\vec{x})V(\vec{r}-\vec{s})f(\vec{r})g(\vec{s})\,d\vec{r}\,d\vec{s}\,.
\end{aligned} \tag{3.3}$$

The functional F_{LS} is just the Hartree approximation for the energy functional. More interesting is F_{TLS}. With Fourier transforms

$$\begin{aligned}
&f(\vec{r}) = (2\pi)^{-3/2}\int e^{i\vec{p}\cdot\vec{r}}\tilde{f}(\vec{p})\,d\vec{p}\,,\\
&V(\vec{r}) = \int e^{i\vec{p}\cdot\vec{r}}\tilde{V}(\vec{p})\,d\vec{p}\,,
\end{aligned} \tag{3.4}$$

it follows that

$$\begin{aligned}
N(\vec{0}) &= (2\pi)^3\int |\tilde{f}(\vec{p})|^2|\tilde{g}(-\vec{p})|^2\,d\vec{p}\,,\\
H(\vec{0}) &= (2\pi)^3\int\left(\frac{p^2}{2M_1}+\frac{p^2}{2M_2}\right)|\tilde{f}(\vec{p})|^2|\tilde{g}(-\vec{p})|^2\,d\vec{p} + (2\pi)^3\int \tilde{f}^*(\vec{p})\tilde{g}(-\vec{p})\tilde{V}(\vec{p}-\vec{q})\tilde{f}(\vec{q})\tilde{g}(-\vec{q})\,d\vec{p}\,d\vec{q}\,.
\end{aligned} \tag{3.5}$$

Let

$$\tilde{\phi}(\vec{p}) = (2\pi)^{3/2}\tilde{f}(\vec{p})\tilde{g}(-\vec{p}), \tag{3.6}$$

so that

$$\begin{aligned}
N(\vec{0}) &= \int |\tilde{\phi}(\vec{p})|^2\,d\vec{p}\,,\\
H(\vec{0}) &= \int \frac{p^2}{2\mu}|\tilde{\phi}(\vec{p})|^2\,d\vec{p} + \int \tilde{\phi}(\vec{p})\tilde{V}(\vec{p}-\vec{q})\tilde{\phi}(\vec{q})\,d\vec{p}\,d\vec{q}\,,\\
&\frac{1}{\mu} = \frac{1}{M_1}+\frac{1}{M_2},
\end{aligned} \tag{3.7}$$

and, therefore, $\tilde{\phi}(\vec{p})$ is just the Fourier transform of the relative two-particle wave function that satisfies the Schrödinger equation

$$\left[-\frac{\nabla^2}{2\mu} + V(\vec{r})\right]\phi(\vec{r}) = \epsilon\,\phi(\vec{r}) \tag{3.8}$$

and

$$E_{\mathrm{TBLS}} = \epsilon\,. \tag{3.9}$$

That is, E_{TBLS} is the correct energy for two particles interacting via the potential V.

Further light on this amusing result is obtained by considering the state

$$|\vec{K}=\vec{0};f,g\rangle=(2\pi)^{-3/2}\int|\vec{x};f,g\rangle d\vec{x}; \tag{3.10}$$

the details are left to the reader.

IV. SHELL MODEL

The Hamiltonian and states $|\vec{x}\rangle$ are given by Eqs. (1.3) and (1.4). In this case it is easy to see that $F_{\mathrm{LS}}\{f_i\}$ is the Hartree-Fock energy functional, so that E_{LS} and f_i^{LS} are the Hartree-Fock energy and single-particle wave functions. In this case E_{TILS} contains the correction for center-of-mass motion originally proposed by Peierls and Yoccoz.[1] The TBLS formulation, which was shown in the previous section to give the correct answer for the two-particle system, seems likely to give interesting results for systems with relatively few particles.

It is interesting to consider various states $|\vec{x};S_\alpha\rangle$, where S_α for varying α are different sets of occupied orbitals. Then $D(\vec{x})$ and $A(\vec{x})$ must be extended to

$$\begin{aligned}D_{\alpha\beta}(\vec{x})&=\langle\vec{x};S_\alpha|\vec{0};S_\beta\rangle,\\ A_{\alpha\beta}(\vec{x})&=\langle\vec{x};S_\alpha|H|\vec{0};S_\beta\rangle.\end{aligned} \tag{4.1}$$

With the usual orthogonality properties, it follows that

$$D_{\alpha\beta}(\vec{0})=\delta_{\alpha\beta}, \tag{4.2}$$

so that the use of just $A_{\alpha\beta}(\vec{0})$ and $D_{\alpha\beta}(\vec{0})$ leads to the usual situation in which configuration interaction is used to improve the Hartree-Fock ground state.

More interesting is the TILS approximation in which the f_i^{LS} from the Hartree-Fock calculation are used to compute $D_{\alpha\beta}(\vec{x})$ and $A_{\alpha\beta}(\vec{x})$ and then

$$\begin{aligned}N_{\alpha\beta}(\vec{0})&=\int D_{\alpha\beta}(\vec{x})d\vec{x},\\ H_{\alpha\beta}(\vec{0})&=\int A_{\alpha\beta}(\vec{x})d\vec{x}.\end{aligned} \tag{4.3}$$

Here the superposition of states α that minimizes $\langle H\rangle/\langle N\rangle$ is computed by choosing λ so that the lowest eigenvalue of

$$H_{\alpha\beta}(\vec{0})-\lambda N_{\alpha\beta}(\vec{0}) \tag{4.4}$$

is zero; then λ is the desired value of $\langle H\rangle/\langle N\rangle$. Excited states can also be calculated. As was noted in Ref. 1, this scheme will eliminate in a natural way the "spurious states" that occur when excited configurations are used in E_{LS}.

The effective mass is simply computed here. Using the G of Sec. II and making the transformation

$$\psi(\vec{r})=e^{iM\vec{v}\cdot\vec{r}}\chi(\vec{r}) \tag{4.5}$$

in H and $\vec{P}$ of Eqs. (1.3) gives

$$\begin{aligned}G&=\int\chi^\dagger(r)\left(-\frac{\nabla^2}{2M}\right)\chi(\vec{r})+\tfrac{1}{2}\int\chi^\dagger(\vec{r})\chi^\dagger(\vec{s})V(\vec{r}-\vec{s})\chi(\vec{s})\chi(\vec{r})d\vec{r}\,d\vec{s}-\tfrac{1}{2}Mv^2\int\chi^\dagger(\vec{r})\chi(\vec{r})d\vec{r},\\ \vec{P}&=M\vec{v}\int\chi^\dagger(\vec{r})\chi(\vec{r})d\vec{r}-i\int\chi^\dagger(\vec{r})\nabla\chi(\vec{r})d\vec{r}.\end{aligned} \tag{4.6}$$

Since the number of particles,

$$A=\int\psi^\dagger(\vec{r})\psi(\vec{r})d\vec{r}=\int\chi^\dagger(\vec{r})\chi(\vec{r})d\vec{r}, \tag{4.7}$$

is a constant, G and $\vec{P}$ for $\vec{v}\neq 0$ differ from G and $\vec{P}$ for $\vec{v}=0$ only by constants. Therefore, the solution $f_i^{\mathrm{LS},\vec{v}}$ is obtained from Eq. (4.5)

$$f_i^{\mathrm{LS},\vec{v}}=e^{-iM\vec{v}\cdot\vec{r}}f_i^{\mathrm{LS},\vec{0}}, \tag{4.8}$$

and since

$$\langle\vec{P}\rangle^{\vec{v}=0}=0, \tag{4.9}$$

it follows that

$$\begin{aligned}\vec{P}_{\mathrm{LS}}(\vec{v})&=AM\vec{v},\\ E_{\mathrm{LS}}(\vec{v})&=G_{\mathrm{LS}}(\vec{v})+\vec{v}\cdot\vec{P}_{\mathrm{LS}}(\vec{v})=E_{\mathrm{LS}}(\vec{0})+\frac{\vec{P}_{\mathrm{LS}}{}^2}{2AM},\end{aligned} \tag{4.10}$$

and

$$M^*=AM, \tag{4.11}$$

as it should be. The same result also holds in the TILS and TBLS approximations. The value M_a^* of Eq. (2.13) was used by Griffin and Wheeler[3] and also in Ref. 1 and gave an incorrect result.

V. POLARON

The Hamiltonian is given by Eq. (1.6). The ψ part of the localized state $|\vec{x}\rangle$ will be as in the shell model. For the phonon part, associated with the boson operators $a(k)$, the coherent state[2] localized at $\vec{x}$ will be used:

$$\begin{aligned}|\vec{x};b\rangle&=W_{\vec{x}}^\dagger\{b\}|\Omega_B\rangle,\\ W_{\vec{x}}^\dagger\{b\}&=\exp\left[-\tfrac{1}{2}\int|b(\vec{k})|^2d\vec{k}\right.\\ &\qquad\left.+\int b(\vec{k})a^\dagger(\vec{k})e^{-i\vec{k}\cdot\vec{x}}d\vec{k}\right],\end{aligned} \tag{5.1}$$

where $|\Omega_B\rangle$ is the phonon vacuum

$$a(\vec{k})|\Omega_B\rangle = 0\,, \quad \text{all } \vec{k}\,. \tag{5.2}$$

Since the $a(\vec{k})$ satisfy Bose commutation relations, it follows that

$$\vec{P}a^\dagger(\vec{k}) = a^\dagger(\vec{k})(\vec{P}+\vec{k})\,,$$

$$e^{-i\vec{P}\cdot(\vec{y}-\vec{x})}a^\dagger(\vec{k}) = a^\dagger(k)e^{-ik\cdot(y-x)}e^{-iP\cdot(y-x)}\,, \tag{5.3}$$

$$e^{-i\vec{P}\cdot(\vec{y}-\vec{x})}W_{\vec{x}}^\dagger\{b\}e^{i\vec{P}\cdot(\vec{y}-\vec{x})} = W_{\vec{y}}^\dagger\{b\}$$

as required by Eq. (1.1). From the form of Eq. (5.1) it follows that

$$[a(\vec{k}), W_{\vec{x}}^\dagger\{b\}] = e^{-i\vec{k}\cdot\vec{x}}b(\vec{k})W_{\vec{x}}^\dagger\{b\} \tag{5.4}$$

so that

$$a(\vec{k})|\vec{x};b\rangle = e^{-i\vec{k}\cdot\vec{x}}b(\vec{k})|\vec{x};b\rangle\,. \tag{5.5}$$

This equation makes the evaluation of matrix elements a simple matter.

The localized coherent state for the polaron is

$$|\vec{x};b,f\rangle = \int \psi^\dagger(\vec{r})f(\vec{r}-\vec{x})d\vec{r}\, W_{\vec{x}}^\dagger\{b\}|\Omega\rangle\,, \tag{5.6}$$

$$a(\vec{k})|\Omega\rangle = 0, \quad \text{all } \vec{k}$$

$$\psi(\vec{r})|\Omega\rangle = 0, \quad \text{all } \vec{r}\,.$$

In this case $D(\vec{x})$ factors into a fermion part and a boson part,

$$D(\vec{x}) = D_B(\vec{x})D_F(\vec{x})\,,$$

$$D_F(\vec{x}) = \int f^*(\vec{r}-\vec{x})f(\vec{r})d\vec{r}\,, \tag{5.7}$$

$$D_B(\vec{x}) = \langle\Omega_B|W_{\vec{x}}\{b\}W_0^\dagger\{b\}|\Omega_B\rangle$$
$$= \exp\left[-\int |b(\vec{k})|^2(1-e^{i\vec{k}\cdot\vec{x}})d\vec{k}\right],$$

and $A(\vec{x})$ is given by

$$A(\vec{x}) = D_B(\vec{x})\int f^*(\vec{r}-\vec{x})\left(-\tfrac{1}{2}\nabla^2 - \frac{\gamma^{1/2}}{2\pi}\int\frac{e^{i\vec{p}\cdot\vec{r}}}{p}[b(\vec{p})+b^*(-\vec{p})e^{-i\vec{p}\cdot\vec{x}}]d\vec{p}\right)f(\vec{r})d\vec{r} + D(\vec{x})\int|b(\vec{k})|^2e^{i\vec{k}\cdot\vec{x}}d\vec{x}\,. \tag{5.8}$$

Now two cases can be distinguished: (a) f has no δ-function part and $A(0)/D(0)$ is meaningful, and (b) f has a δ-function part so that $A(\vec{x}) \propto \nabla^2\delta(\vec{x})$ and $D(\vec{x}) \propto \delta(\vec{x})$ and therefore $A(0)/D(0)$ is not meaningful.

Consider the first of these. Since $D_B(0) = 1$, it follows that

$$F_{\rm LS}\{b,f\} = \int f^*(\vec{r})\left(-\tfrac{1}{2}\nabla^2 - \frac{\gamma^{1/2}}{2\pi}\int\frac{e^{i\vec{k}\cdot\vec{r}}}{k}[b(\vec{k})+b^*(-\vec{k})]d\vec{k} + \int|b(\vec{k})|^2d\vec{k}\right)f(\vec{r})d\vec{r}\,, \tag{5.9}$$

where $f(\vec{r})$ is required to satisfy the condition

$$\int|f(\vec{r})|^2d\vec{r} = 1\,.$$

Then the equation for $b_{\rm LS}(\vec{k})$ is

$$\frac{\delta F_{\rm LS}}{\delta b^*(k)} = 0 = b_{\rm LS}(\vec{k}) - \frac{\gamma^{1/2}}{2k}\int e^{-i\vec{k}\cdot\vec{r}}|f(\vec{r})|^2d\vec{r}\,. \tag{5.10}$$

Substitution gives the LS energy functional

$$F_{\rm LS}\{f\} = \int f^*(\vec{r})\left(-\frac{\nabla^2}{2}\right)f(\vec{r})d\vec{r} - \frac{\gamma}{4\pi^2}\int\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{k^2}|f(\vec{r})|^2|f(\vec{r}')|^2d\vec{r}\,d\vec{r}'$$
$$= \int f^*(\vec{r})\left(-\frac{\nabla^2}{2}\right)f(\vec{r})d\vec{r} - \frac{\gamma}{2}\int|f(\vec{r})|^2\frac{1}{|\vec{r}-\vec{r}'|}|f(\vec{r}')|^2d\vec{r}\,d\vec{r}'\,. \tag{5.11}$$

This is the usual "strong-coupling" expression for the energy functional, which was first given by Pekar.[4] It has the solution

$$E_{\rm LS} = -0.054\gamma^2 = -0.109\alpha^2\,. \tag{5.12}$$

Now suppose that

$$f(\vec{r}) = \delta(\vec{r})\,. \tag{5.13}$$

Then

$$D(\vec{x}) = \delta(\vec{x})$$
$$A(\vec{x}) = -\tfrac{1}{2}D_B(\vec{x})\nabla^2\delta(\vec{x}) + \left(\int|b(\vec{k})|^2d\vec{k} - \frac{\gamma^{1/2}}{2\pi}\int[b(\vec{k})+b^*(-\vec{k})]\frac{d\vec{k}}{k}\right)\delta(\vec{x})\,. \tag{5.14}$$

The functional $F_{\rm LS}$ does not exist, but $F_{T\rm LS}$ is easily obtained from

$$N(\vec{0})=1\,,$$
$$H(\vec{0})=-\tfrac{1}{2}\nabla^2 D_B(\vec{x})\big|_{\vec{x}=0}+\int |b(\vec{k})|^2 dk-\frac{\gamma^{1/2}}{2\pi}\int [b(\vec{k})+b^*(-\vec{k})]\frac{d\vec{k}}{k} \tag{5.15}$$
$$=\int\left(\frac{k^2}{2}+1\right)|b(\vec{k})|^2 d\vec{k}-\frac{\gamma^{1/2}}{2\pi}\int [b(\vec{k})+b^*(-\vec{k})]\frac{d\vec{k}}{k}\,,$$

so that

$$b_{\mathrm{TBLS}}(\vec{k})=\frac{\gamma^{1/2}}{2k(1+\frac{1}{2}k^2)}$$
$$E_{\mathrm{TBLS}}=-\frac{\gamma}{4\pi^2}\int\frac{d\vec{k}}{k(1+\frac{1}{2}k^2)}=-\frac{\gamma}{\sqrt{2}}=-\alpha\,, \tag{5.16}$$

which is the usual "weak-coupling" result.

In this case, it follows that the TBLS approximation will give the weak-coupling result if the range of $f(r)$ is much smaller than the logarithmic derivative of $D_B(x)$. It must always give an energy that satisfies

$$E_{\mathrm{TBLS}}\leq-\alpha\,, \tag{5.17}$$

where the equality holds only for $\alpha=0$. Of course, since $E_{\mathrm{TBLS}}<E_{\mathrm{LS}}$, it follows that E_{TBLS} is necessarily less than the usual strong-coupling energy.

It is interesting to note that $\alpha=0$ is a singular point in this approximation in a novel way. That is, the singularity is in the extent of the function $f(r)$; this extent goes to zero as α and γ go to zero. This sort of singularity might well explain the singularities that occur in other quantum field theories.

VI. SUMMARY

The translated-localized-state methods discussed in this paper have been shown to give exact results for the two-body problem and to give a simple way of understanding the connection between strong and weak coupling in the polaron. The apparent discrepancy in the shell-model effective mass described in Refs. 1 and 3 was shown to be illusory; the translated-localized-state methods give the exact answer in the case of many particles interacting via two-body forces.

The TBLS method of Sec. II is simple to use in the case of the weak-coupling polaron. However, it appears promising for the polaron in general and for light nuclear systems.

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