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Multicomponent polaron

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By a slight modification of the Fröhlich Hamiltonian (the introduction of an internal quantum number) we reduce the polaron problem to the solution of a continued fraction, even at finite temperature. We analyze both the stationary states and the resonances (in one- and three-dimensional versions of the model) and exhibit some unexpected results.

INTRODUCTION

Despite half a century of efforts, Fröhlich's model[1] of a slow electron in a polar medium remains only partially solved to this day. However, we have found that a slight modification produces a model, the exact solution of which leads to two-coupled, nonlinear integrodifference equations with which to construct the eigenstates. Our modification consists of adding an internal quantum number $\sigma=1,2,\ldots,\infty$ labeling the internal state of the fermion and the bosons with which it interacts. The model Hamiltonian is

$$H=\sum_{\sigma,\mathbf{k}}k^2c^*_{\sigma,\mathbf{k}}c_{\sigma,\mathbf{k}}-\sum_{\sigma,\mathbf{q}}[V_\sigma(\mathbf{q})a^*_{\sigma,\mathbf{q}}c^*_{\sigma+1,\mathbf{k}-\mathbf{q}}c_{\sigma,\mathbf{k}}+\text{H.c})]+\sum_{\sigma,\mathbf{q}}\hbar\omega_\mathbf{q}a^*_{\sigma,\mathbf{q}}a_{\sigma,\mathbf{q}}\ , \quad (1)$$

in which the c's are electron (fermion) operators ($\hbar^2/2m=1$) and the a's are optical-phonon (boson) operators, all in a box of volume $L^3\to\infty$.

With $\mathbf{k},\mathbf{q}$ unrestricted, the lowest-lying eigenstates—the so-called "large polaron"[2] states—are labeled by the quantum number σ and momentum $\mathbf{k}$:

$$|\sigma,\mathbf{k}\rangle=c^*_{\sigma,\mathbf{k}}|0\rangle+\sum_\mathbf{q}F(\mathbf{q};\mathbf{k})c^*_{\sigma+1,\mathbf{k}-\mathbf{q}}a^*_{\sigma,\mathbf{q}}|0\rangle+\sum_\mathbf{q}\sum_{\mathbf{q}'}F(\mathbf{q},\mathbf{q}';\mathbf{k})c^*_{\sigma+2,\mathbf{k}-\mathbf{q}}a^*_{\sigma+1,\mathbf{q}'}a^*_{\sigma,\mathbf{q}}|0\rangle+\cdots\ . \quad (2)$$

The corresponding energy eigenvalues are

$$E_\sigma(\mathbf{k})=k^2-\sum_\mathbf{q}F(\mathbf{q};\mathbf{k})V_\sigma(\mathbf{q})^*\ . \quad (3)$$

The interactions V_σ could be allowed to depend on σ. For example, if one sets all $V_\sigma\equiv0$ for $\sigma\geq2$ and retains $V_1(\mathbf{q})$ as the only nonzero interaction potential, the model formally reduces to an easily solved, asymmetric variant of the "magnetic polaron," in which an electron with spin (here, $\sigma=1$ and 2) interacts with the magnetic background by the emission or absorption of magnons (here $a_{1,\mathbf{q}},a^*_{1,\mathbf{q}}$). Its analysis is left as an exercise for the reader. In a somewhat less trivial, rotationally invariant SU(2) version, this model has long ago been solved explicitly, and has found a number of physical applications to magnetic semiconductors.[3]

In the present paper, we allow for an *infinite* number of internal states, taking the $V_\sigma(\mathbf{q})$ to be independent of σ for $\sigma=1,2,\ldots,\infty$. Thus electronic states are infinite-dimensional spinors accompanied by the corresponding bosons. Even in this case the model reduces to quadrature for arbitrary potentials $V(\mathbf{q})$ and arbitrary phonon dispersion $\omega_\mathbf{q}$. In order to make contact with the standard models and approximations,[4] we have specialized in the Fröhlich interaction $V(\mathbf{q})=[4\pi\alpha/(q^2L^3)]^{1/2}$ in the three-dimensional (3D) model, and taken the phonon energy $\hbar\omega_\mathbf{q}=1$ to be a constant defining the unit of energy. Additionally, we examine an even simpler, one-dimensional version in which the interaction potential is a δ function, i.e., $V(\mathbf{q})=$constant.

EIGENSTATES OF H_t

We solve the Schrödinger equation $H|\sigma,\mathbf{k}\rangle=E(\mathbf{k})|\sigma,\mathbf{k}\rangle$, by equating coefficients of the various configurations:

$$c^*_{\sigma,\mathbf{k}}|0\rangle,c^*_{\sigma+1,\mathbf{k}-\mathbf{q}}a^*_{\sigma,\mathbf{q}}|0\rangle,c^*_{\sigma+2,\mathbf{k}-\mathbf{q}}a^*_{\sigma+1,\mathbf{q}'}a^*_{\sigma,\mathbf{q}}|0\rangle,\ \text{etc}\ .$$

The first result is Eq. (3), the second yields $F(\mathbf{q};\mathbf{k})$:

$$F(\mathbf{q};\mathbf{k})=-V(\mathbf{q})/[E(\mathbf{k})-(\mathbf{k}-\mathbf{q})^2-1-\Sigma(\mathbf{k}-\mathbf{q};E(\mathbf{k})-1)]\ ,$$
$$F(\mathbf{q},\mathbf{q}';\mathbf{k})=-F(\mathbf{q};\mathbf{k})\mathrm{V}(\mathbf{q}')/[E(\mathbf{k})-(\mathbf{k}-\mathbf{q}-\mathbf{q}')^2-2-\Sigma(\mathbf{k}-\mathbf{q}-\mathbf{q}';E(\mathbf{k})-2)],\ \text{etc.}\ , \quad (4)$$

where

$$\Sigma(\mathbf{k};\omega)\equiv\sum_\mathbf{q}V^2(\mathbf{q})/[\omega-(\mathbf{k}-\mathbf{q})^2-1-\Sigma(\mathbf{k}-\mathbf{q};\omega-1)]\ . \quad (5)$$

This equation, or variants thereof, has often been seen before.[5–7] For example, Eq. (5) expresses the self-energy of the Fröhlich polaron in the Hartree (i.e., the random-phase approximation[5,6]). Whitfield and Puff[6] assumed a functional form $\Sigma(\mathbf{k};\omega)=a(\omega)+k^2b(\omega)$ and, taking $k\rightarrow 0$, solved numerically for the functions $a(\omega),b(\omega)$. However, their ansatz can be correct only for special interactions (such as the δ function we shall examine in 1D) and therefore we do not make use of it at present.

We use (5) to rewrite (3) as an implicit equation in $E(\mathbf{k})$:

$$E(\mathbf{k})=k^2+\Sigma(\mathbf{k};E(\mathbf{k})) . \tag{6}$$

Once $\Sigma(\mathbf{k};\omega)$ is found in Eq. (5), Eq. (6) fixes the eigenvalue $E(\mathbf{k})$ and Eq. (4) determines the amplitudes $F(\mathbf{q};\mathbf{k})$, $F(\mathbf{q},\mathbf{q}';\mathbf{k}), \ldots$ for the eigenstates, Eqs. (2).

GENERALIZATION TO FINITE TEMPERATURE

There have been several studies of the effects of finite T on the properties of the polaron, notably by Dunn.[8] In the present model, the equations for the eigenstates are easily generalized to finite T by the use of thermal Green functions. The equations of motion of the retarded Green function[9] yield

$$G(\mathbf{k},\omega)=(1/2\pi)/[\omega-(\mathbf{k}-\mathbf{q})^2-\Sigma_T(\mathbf{k}-\mathbf{q};\omega-1)] , \tag{7}$$

where

$$\Sigma_T(\mathbf{k};\omega)=\sum_{\mathbf{q}} V^2(\mathbf{q})[1+n(T)]/[\omega-(\mathbf{k}-\mathbf{q})^2-1-\Sigma_T(\mathbf{k}-\mathbf{q};\omega-1)] , \tag{8}$$

with $n(T)=1/[\exp(1/k_BT)-1]$, is a trivial generalization of (5). With a little more effort than what is required to obtain $E(\mathbf{k})$, one can calculate the thermal expectation value of the interaction Hamiltonian with the aid of this G and consequently, the excess *free energy* of a composite particle. We intend to pursue this interesting generalization in the future.

SELF-CONSISTENT SOLUTION OF $\Sigma(\mathbf{k},\omega)$

Converting (5) to an integral and shifting the origin to $\mathbf{k}$ one obtains:

$$\Sigma(k;\omega)\equiv L^3\int d^3q\,(2\pi)^{-3}V^2(\mathbf{q}-\mathbf{k})/[\omega-q^2-1-\Sigma(q;\omega-1)]$$
$$=(\alpha/\pi)k^{-1}\int_0^\infty dq\, q\ln|(q+k)/(q-k)|/[\omega-q^2-1-\Sigma(q;\omega-1)] . \tag{9}$$

Because $\Sigma(k;\omega)$ depends on $k=|\mathbf{k}|$ and ω only, the originally four-dimensional problem reduces to two dimensions. Still, (9) represents two-coupled, nonlinear, integrodifference equations, one for the real part $R(k,\omega)$ of $\Sigma(k;\omega)$ and the other for its imaginary part $I(k,\omega)$. Causality requires $I(k,\omega)\geq 0$. For computational purposes, we created a two-dimensional grid of some 20 000 points over the relevant range of k and ω, and numerically solved for the real and imaginary parts of Σ on this grid by iteration, until graphical accuracy [O(1%)] was achieved.

We list salient features of the solutions, some of which are shared with the Fröhlich model:[4-8]

(1) Stationary states exist only for $|k|<k_c$, where k_c, a function of α, is defined by

$$E(k_c)-E(0)=1 \tag{10}$$

and is the threshold for emitting a phonon. This implies a minimum radius $\approx\pi/k_c(\alpha)$ for the stable polaron. All states carrying momentum $|k|>k_c$ decay in time, more or less rapidly depending on the magnitude of $I(k,\omega)$.

Figure 1 shows graphically the solution of Eq. (6) at $k=0$, $\alpha=1$: $E(0)=R(0,E(0))$. One solution corresponds to $E<0$ and is a stationary state [i.e., $I(0,E(0))=0$] but others are found at $E>0$ with $I(0,E)\neq 0$, and are classified as finite-lived resonances which are better described in the time-dependent Schrödinger equation formalism than as eigenstates. In the example of Fig. 1, we see one bound state and one resonance only. The resonance could be a numerical artifact, as the height of the peaks in $R(k,\omega)$ is sensitive to numerical accuracy and mesh size. Moreover, because $I(k,\omega)$ goes from steep maxima to shallow minima over small ranges of energies, at some special k's the resonance can attain comparatively very long lifetime, during which it behaves as a bound state (while technically remaining part of the continuum of scattering states). For other ranges of k, there may be no resonant states whatsoever (which means that all excited states at those k's are overdamped, to the extent that they have no characteristic energy). We shall see examples of both extremes in the one-dimensional example which follows.

(2) Near a true bound-state solution we find $I(0,E(k)+\delta\omega)$ vanishes at *all* $\delta\omega<0$, then rises to a large peak beyond some positive threshold for $\delta\omega$.

(3) The spectral intensity function $A(k,\omega)$, obtained from the $T\rightarrow 0$ Green function, is also shown in Fig. 1. It reflects the bound state at $\omega=E(k)$ as a sharp peak, followed by peaks at $E(k)+1, E(k)+2, \ldots$. While the first of these has been identified as a resonance, the others are merely incoherent scattering states of the composite particle in the presence of $2,3,\ldots,$ phonons.

Figure 2 shows the ground-state energy as a function of α. Its inset shows the dispersion, computed at $\alpha=3$. While the ground-state energy is accurately given, present accuracy is insufficient to exhibit the expected[6,8] flattening of the dispersion at k_c [i.e., $\partial E/\partial(k^2)|_c=0$.] (The figure also indicates some numerical "jitter.") A planned increase in the number of points leading to a decrease in mesh size by a factor of 10 or more should cure all numerical problems. But we now turn to a one-dimensional version, for which the present accuracy is amply sufficient.

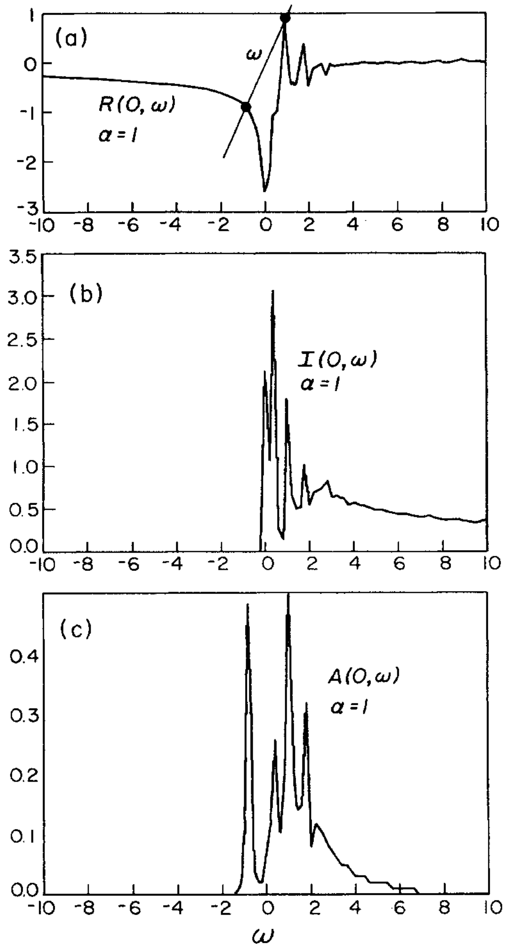

FIG. 1. Graphical solution of Eq. (6) at $\mathbf{k}=0$, for $\alpha=1$. Top panel shows two intersections of ω and $R(0;\omega)\equiv\mathrm{Re}[\Sigma(0;\omega)]$, middle panel shows that the leftmost intersection has $I(0;\omega)\equiv\mathrm{Im}[\Sigma(0;\omega)]=0$; hence the corresponding state is an energy eigenstate. (The rightmost intersection is a resonance.) The first two peaks in the Green-function spectral intensity $A(0;\omega)$ (lowest panel) correspond to the bound and resonant states, respectively, while the higher peaks have no physical significance.

A SOLVABLE MODEL IN 1D

The one-dimensional version of our model can almost be solved in closed form. With the interaction a δ function in space, $V(q)=(2\alpha/L)^{1/2}$ is independent of q. The analog to Eq. (9) is

$$\Sigma(k;\omega)=(\alpha/\pi)\int_{-\infty}^{+\infty}dq[\omega-q^2-1-\Sigma(q;\omega-1)]^{-1} \quad (11)$$

normalized to coincide with the right-hand side of Eq. (9) in $\lim_{k\to 0}$. In this instance, a Whitfield-Puff-type[6] ansatz is, in fact, justified as $\Sigma(k;\omega)$ can be written $\Sigma(\omega)=R(\omega)+iI(\omega)$, with both R and I real functions of ω independent of k, with $I\geq 0$. The integral is easily evaluated to yield a continued fraction

$$\Sigma(\omega)=-\alpha/[1-\omega+\Sigma(\omega-1)]^{1/2} . \quad (12)$$

The graphical solution of the eigenvalue equation for

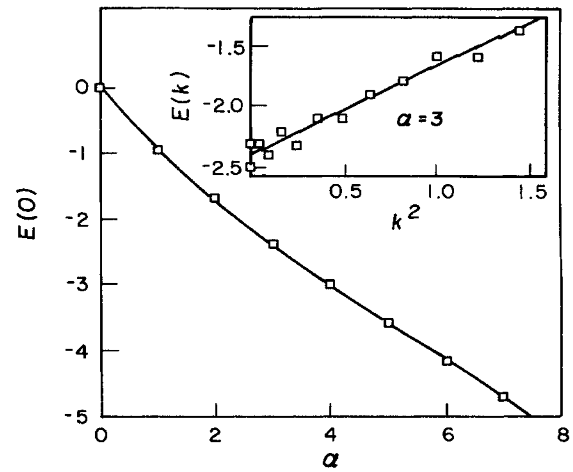

FIG. 2. Ground-state energy $E(\mathbf{0})$ vs coupling constant α. Inset: shows dispersion (E vs k^2) at $\alpha=3$. The approximately linear relation indicates that the effective-mass approximation is fairly accurate over the range of energy for which the composite particle exists.

bound states

$$k^2=E(k)-R(E(k)) \text{ and } I(E(k))=0 , \quad (13)$$

is illustrated in Fig. 3 for a typical intermediate-coupling value $\alpha=3$. From the small k behavior, we can obtain the effective mass, $m^*/m=1-\partial R(E)/\partial E|_{E(k)}$; it is plotted as a function of α in the same figure. From Fig. 3, it appears obvious that a bound state exists at any k, and thus that $k_c=\infty$. This is a consequence of the inverse-square-root nature of the divergence[10] of $R(\omega)$ at $\omega=E(0)+1$ seen in Fig. 3. Its behavior can be related to α and m^* by combining (12) and (13) as follows:

$$\lim_{\delta\omega\to 0^+}[R(E(0)+1-\delta\omega)]=-\alpha/(m^*\delta\omega/m)^{1/2}\to\infty . \quad (14)$$

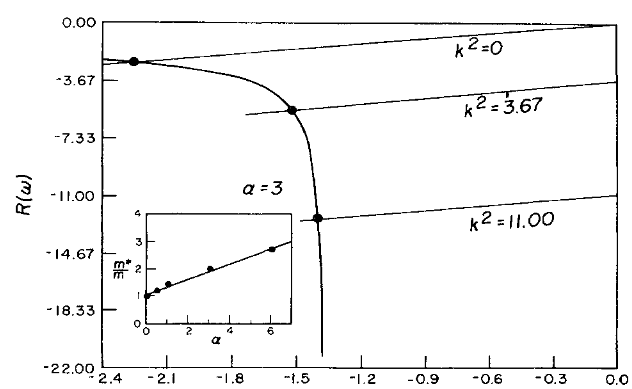

FIG. 3. One-dimensional model: graphical solution of Eq. (13) at various k for the particular example $\alpha=3$. [Ground-state energy $E(0)$ vs α is essentially the same as in 3D, as already plotted in Fig. 2.] From small k^2 behavior we can extract m^*/m at each α. Inset: m^*/m vs α (five calculated points; the straight line is just a guide to the eye).

The excited states (resonances) in 1D can also be completely catalogued, by an extension of the analysis to all ω and of $\Sigma(\omega)$ into the complex domain. At any α, for the range of energies $E(0) \leq E(k) < E(0)+1$, there are only bound states. What happens in the next range of energies will be described as follows.

(4) $E(0)+1 \leq E_{\text{exc}}(k) < E(0)+2$, there is *no* resonance whatever. This surprising result implies that all excited states carrying momentum $|k| < \sqrt{[2+E(0)]}$ rapidly decay to the ground-state polaron.

(5) *Precisely* at $|k| = \sqrt{[2+E(0)]}$ (where the excited-state energy has the value $E_{\text{exc}} = E(0)+2$), we discover an infinitely sharp resonance: a true eigenstate, within the continuum. This "accidental" eigenstate is the consequence of $I(\omega)$ having a cusp and vanishing at precisely this energy. There are no other, higher, resonant states at this special value of $|k|$.

(6) For $|k| > \sqrt{[2+E(0)]}$ there is one (occasionally, two) resonance of finite width at each k, gradually broadening with increasing $|k|$.

To within graphical accuracy, the dependence of the ground-state energy $E(0)$ on α in the 1D model agrees with the curve we computed separately for 3D over the entire range of α shown in Fig. 2. In both instances, the energies are continuous functions of α and there is no itinerant-to-localized phase transition for these potentials. This agrees with the findings of Peeters and Devreese[11] concerning the absence of a phase transition in the Fröhlich model. The principal differences between our 1D and 3D models are to be found at large k, and concern such delicate issues as the existence of a cutoff $k_c(\alpha)$ in 3D but not in 1D.

ACKNOWLEDGMENTS

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[1] H. Fröhlich, H. Pelzer, and S. Zienau, Philos. Mag. **41**, 221 (1950). The original concept can be dated back to L. D. Landau, Z. Phys. Sowjetunion, **3**, 664 (1933). Well-known calculations include those of S. Pekar, J. Phys. **10**, 347 (1946); R. P. Feynman, Phys. Rev. **97**, 660 (1955); T. D. Schultz, *ibid.* **116**, 526 (1959); T. D. Lee and D. Pines, *ibid.* **92**, 883 (1955); J. M. Luttinger and C.-Y. Lu, *ibid.* **21**, 4251 (1980).

[2] They are referred to as large polaron states in order to distinguish them from the "small polaron," in which **q**, **k** are restricted to the first Brillouin zone. (The small polaron can also be solved in our model.) Also, see Ref. 4.

[3] See S. Methfessel and D. C. Mattis, *Magnetic Semiconductors,* Vol. XVIII/1 of *Handbuch der Physik,* edited by S. Flügge (Springer-Verlag, Berlin, 1968), pp. 389–562 (especially pp. 419–423) for a solution later extended and amplified by B. S. Shastry and D. C. Mattis, Phys. Rev. B **24**, 5340 (1981). The t-J model requires, for its approximate solution, *two* internal states: one for each magnetic sublattice. See D. C. Mattis and H. Chen, Int. J. Mod. Phys. B **5**, 1401 (1991).

[4] For more information on the usual polaron models see T. K. Mitra, A. Chatterjee, and S. Mukhopadhyay, Phys. Rep. **153**, 91 (1987), which also supplies a reasonably complete bibliography; also the monograph by N. N. Bogoliubov and N. N. Bogoliubov, Jr., *Some Aspects of Polaron Theory* (World Scientific, Singapore, 1988). The most recent calculations based on Feynman's solution of the Fröhlich model are described in a brief review by C. Alexandrou, W. Fleischer, and R. Rosenfelder, Mod. Phys. Lett. B **5**, 613 (1991).

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[6] G. Whitfield and R. Puff, Phys. Rev. **139**, A338 (1965); D. M. Larsen, Phys. Rev. **144**, 697 (1966); F. M. Peeters, P. Warmenbol, and J. T. Devreese, Europhys. Lett. **3**, 1219 (1987), find that similar analysis in 2D produces quite different results (but not unlike what we have found in 1D).

[7] Equation (7) also has analogs in the many-body perturbation theory.

[8] D. Dunn, Can. J. Phys. **53**, 321 (1975).

[9] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [Sov. Phys. Usp. **3**, 320 (1960)].

[10] In 3D, by way of comparison, the threshold is also at one phonon energy above $E(0)$, but the corresponding integral Eq. (9) is finite at threshold. Therefore k_c is finite, a function of α.

[11] F. M. Peeters and J. T. Devreese, Phys. Status Solidi B **112**, 219 (1982).