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Resolution of the Runaway Problem for the Polaron

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Runaway modes are shown to result from the standard application of the dipole approximation to the polaron Hamiltonian. These modes do not occur if the Hamiltonian is renormalized before making the approximation.

I. INTRODUCTION

EXACTLY solvable model-field theories whose Hamiltonians are quadratic in the dynamical variables have long been known to suffer from renormalization-induced runaway modes.¹⁻⁴ These runaway modes—solutions of the equations of motion which display exponential time development—arise because the renormalization prescription employed transforms the originally positive-definite Hamiltonian into an indefinite operator which admits imaginary eigenvalues.

The techniques^{2,5} which have been developed for treating the runaway modes are essentially analogs of the classical prescription, which removes them by imposing boundary conditions.⁶ In the quantum case these modes are simply not included in the eigenfunction expansion of the field operators. This truncation leads to a non-causal theory, as is easily seen by examining the resultant field commutators. These take the characteristic form

$$[\phi(\mathbf{x}), \pi(\mathbf{y})] = i[\delta(\mathbf{x}-\mathbf{y}) - f(\mathbf{x})f(\mathbf{y})], \quad (1)$$

where $f(\mathbf{x})$ is the wave function for the runaway mode. This loss of causality has not been considered to be drastic because the spatial extent of the runaway mode is of the order of 10^{-13} cm about the source. Also, there is no radiation associated with it.

However, if Hamiltonian dynamics is to be considered

a self-consistent system, there is no room for an *ad hoc* prescription for the removal of runaway modes or for the resulting noncausality of the remaining theory. Thus, the following suggestions for the resolution of the runaway problem have been made:

(i) This class of Hamiltonians is either non-Hermitian or does not have eigenstates, and by insisting upon their existence the runaways appear⁷; or

(ii) this class of Hamiltonians is not essentially self-adjoint, and if the deficiency indices are equal, the self-adjoint extensions should be taken as the correct Hamiltonians.⁸

A simpler alternative solution to the runaway problem is suggested by the fact that the runaways are not solutions to the equations of motion generated by the full translationally invariant Hamiltonian. Thus, one is led to conjecture that the runaway modes result from an improper application of the dipole approximation which alters the dynamics of the system in too drastic a manner. In fact, it has long been recognized⁹ that the dipole approximation should only be performed after renormalization, i.e., after the proper field attached to the source has been separated from the external field.

This point of view is further reinforced by the non-uniqueness of the dipole approximation as a result of its noncommutation with canonical transformations. Thus, the many canonically equivalent forms of a translationally invariant Hamiltonian give rise to different dipole approximate forms. Clearly, all of these will not give reasonable approximations to the full dynamics. The

¹ G. Wentzel, *Helv. Phys. Acta* **15**, 111 (1942).

² N. G. Van Kampen, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **26**, No. 15 (1951).

³ H. Steinwedel, *Ann. Physik* **15**, 207 (1955).

⁴ K. Wildemuth and K. Baumann, *Nucl. Phys.* **3**, 612 (1957).

⁵ R. Norton and W. K. R. Watson, *Phys. Rev.* **116**, 1597 (1959).

⁶ P. A. M. Dirac, *Proc. Roy. Soc. (London)* **167**, 148 (1938).

⁷ W. C. Hennenberger, *Nucl. Phys.* **49**, 321 (1963).

⁸ J. M. Jauch, *Math. Rev.* **28**, No. 5716, 1098 (1964).

⁹ M. Schwartz, *Phys. Rev.* **123**, 1903 (1961).

establishment of general criteria is presently under study.

In this paper the dipole approximation is applied to the polaron model in order to illustrate the above conjectures. In Sec. II a canonical transformation is used to cast the polaron model into a form which is similar to the Hamiltonian for nonrelativistic quantum electrodynamics. When the dipole approximation is made and the resulting quadratic Hamiltonian is diagonalized and renormalized, the runaway modes appear.

In Sec. III the canonical transformation which renormalizes the polaron model¹⁰ is made. With the Hamiltonian in this form the dipole approximation yields no runaways upon diagonalization and renormalization.

In Sec. IV the implications of these results for other field-theory models with similar structure are discussed.

II. POLARON HAMILTONIAN

The polaron Hamiltonian, which describes the coupling between a nonrelativistic particle (spinless electron) and a second-quantized scalar field (phonons), is

$$H = \frac{\mathbf{P}^2}{2M_0} + \frac{1}{2} \int d^3k [\omega(k)^2 \phi(\mathbf{k})\phi(-\mathbf{k}) + \pi(\mathbf{k})\pi(-\mathbf{k})] + g \int d^3k \rho(k) \phi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{Q}}. \quad (2)$$

The canonical commutation rules are the usual ones, and the point-source limit is obtained by setting the form factor $\rho(k)$ to unity.

If the dipole approximation were to be made at this stage, the resulting Hamiltonian would just be that of a shifted harmonic oscillator. Clearly, this would be a misuse of the dipole approximation since no electron-phonon scattering would then be included.

This Hamiltonian is cast into the same form as those discussed in the Introduction by the canonical transformation generated by

$$U = \exp \left[-ig \int d^3k \frac{\pi(\mathbf{k})\rho^*(k)}{\omega(k)} e^{-i\mathbf{k}\cdot\mathbf{Q}} \right]. \quad (3)$$

The transformed operators are

$$U\phi(\mathbf{k})U^{-1} = \phi(\mathbf{k}) - g \frac{\rho^*(k)}{\omega(k)^2} e^{-i\mathbf{k}\cdot\mathbf{Q}}, \quad (4)$$

$$UPU^{-1} = \mathbf{P} - ig \int d^3k \mathbf{k} \frac{\rho^*(k)}{\omega(k)^2} \pi(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{Q}}, \quad (5)$$

¹⁰ E. P. Gross, Ann. Phys. (N. Y.) 19, 219 (1962).

and the transformed Hamiltonian is

$$UHU^{-1} = \frac{1}{2} \int d^3k [\omega(k)^2 \phi(\mathbf{k})\phi(-\mathbf{k}) + \pi(\mathbf{k})\pi(-\mathbf{k})] + \frac{1}{2M_0} \left[\mathbf{P} - ig \int d^3k \mathbf{k} \frac{\rho^*(k)}{\omega(k)^2} \pi(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{Q}} \right]^2 - \frac{1}{2} g \int d^3k \frac{|\rho(k)|^2}{\omega(k)^2}. \quad (6)$$

This new Hamiltonian is now reduced to a quadratic form by performing the dipole approximation which removes all particle recoil. Mass renormalization then results by decoupling the field and particle degrees of freedom with the canonical transformation generated by

$$U = \exp \left[\frac{g}{M_r} \int d^3k \mathbf{k} \cdot \mathbf{P} \frac{\rho^*(k)}{\omega(k)^2} \phi(\mathbf{k}) \right], \quad (7)$$

where the renormalized mass M_r is given by

$$M_r = M_0 \left[1 + \frac{g^2}{3M_0} \int d^3k \frac{k^2}{\omega(k)^4} |\rho(k)|^2 \right]. \quad (8)$$

In the point-source limit the bare mass must be taken to be negatively divergent if the renormalized mass is to be finite. This causes the Hamiltonian to take an indefinite form when expressed in terms of the renormalized mass and, thus, leads to runaway modes.

The remaining pair Hamiltonian is

$$UHU^{-1} = \frac{\mathbf{P}^2}{2M_r} + \frac{1}{2} \int d^3k [\omega(k)^2 \phi(\mathbf{k})\phi(-\mathbf{k}) + \pi(\mathbf{k})\pi(-\mathbf{k})] - \frac{g^2}{2M_0} \left[\int d^3k \mathbf{k} \frac{\rho^*(k)}{\omega(k)^2} \pi(\mathbf{k}) \right]^2 - \frac{1}{2} g^2 \int d^3k \frac{|\rho(k)|^2}{\omega(k)^2}, \quad (9)$$

where the operator transformations are

$$U\pi(\mathbf{k})U^{-1} = \pi(\mathbf{k}) - \frac{ig}{M_r} \frac{\rho^*(k)}{\omega(k)^2} \mathbf{k} \cdot \mathbf{P}, \quad (10)$$

$$U\mathbf{Q}U^{-1} = \mathbf{Q} - \frac{ig}{M_r} \int d^3k \mathbf{k} \frac{\rho^*(k)}{\omega(k)^2} \phi(\mathbf{k}). \quad (11)$$

In order to find the runaway modes it is first necessary to diagonalize¹¹ the quadratic in the field operators. The resulting scattering states in momentum space are

$$\Phi_{(\pm)}(\mathbf{k}, \mathbf{p}) = \frac{1}{[2\omega(k)]^{1/2}} \times \left[\delta(\mathbf{k} - \mathbf{p}) + \frac{g^2 \rho(p)\rho^*(k)}{M_0 \omega(p)\omega(k)} \frac{\mathbf{k} \cdot \mathbf{P}}{k^2 - p^2 \mp i\epsilon} \frac{1}{D_{\pm}(k^2)} \right], \quad (12)$$

¹¹ J. M. Blatt, Phys. Rev. 72, 461 (1947).

where

$$D_{\pm}(k^2) = 1 + \frac{g^2}{3M_0} \int d^3p \frac{|\rho(p)|^2}{\omega(p)^2} \frac{p^2}{p^2 - k^2 \mp i\epsilon}. \quad (13)$$

As is well known,¹² there are bound states at the roots of the equation

$$D(k^2) = 1 + \frac{g^2}{3M_0} P \int d^3p \frac{|\rho(p)|^2}{\omega(p)^2} \frac{p^2}{p^2 - k^2} = 0. \quad (14)$$

In terms of the renormalized mass this condition becomes

$$1 + \frac{g^2}{3M_r} \omega(k)^2 P \int d^3p \frac{|\rho(p)|^2}{\omega(p)^2} \frac{p^2}{p^2 - k^2} = 0, \quad (15)$$

and in the point-source limit (with μ set to zero for convenience) adds the imaginary solutions

$$\omega(k) = \pm i3M_r/2\pi^2g^2 \quad (16)$$

which are just the runaway modes.

These results have also been obtained by explicitly expanding the exponential recoil factor in the original form of the Hamiltonian and retaining only quadratic terms after performing a static shift in the field operators.¹³

III. RENORMALIZED FORM

The renormalized form of the Hamiltonian is obtained by performing the canonical transformation which explicitly separates the external and proper fields. In the Hamiltonian this transformation has two effects: The divergent self-energy of the source is explicitly separated out, and the form factor for the charge distribution is modified so as to suppress high-momentum contributions.

In terms of Bose operators the generator of the renormalization transformation is¹⁰

$$U = \exp \left\{ \int d^3k [a(\mathbf{k})\beta(k)^* e^{i\mathbf{k}\cdot\mathbf{Q}} - \text{H.c.}] \right\}, \quad (17)$$

where

$$\beta(k) = -g \frac{\rho^*(k)}{[2\omega(k)]^{1/2}} \Omega(k)^{-1} \quad (18)$$

and

$$\Omega(k) = \omega(k) + k^2/2M_0. \quad (19)$$

The transformed operators are

$$Ua(\mathbf{k})U^{-1} = a(\mathbf{k}) + \beta(k)e^{-i\mathbf{k}\cdot\mathbf{Q}}, \quad (20)$$

$$UPU^{-1} = \mathbf{P} - \int d^3k [a(\mathbf{k}) + \beta(k)\mathbf{k}e^{-i\mathbf{k}\cdot\mathbf{Q}} + \text{H.c.}], \quad (21)$$

and the transformed Hamiltonian is

$$\begin{aligned} UHU^{-1} &= \frac{\mathbf{P}^2}{2M_0} + \int d^3k \omega(k)a(\mathbf{k}) + a(\mathbf{k}) \\ &+ \frac{1}{2M_0} \int d^3p \int d^3q \mathbf{p}\cdot\mathbf{q}\beta(p)^*\beta(q)^* e^{-i(\mathbf{p}+\mathbf{q})\cdot\mathbf{Q}} \\ &\times [a(\mathbf{p}) + a(\mathbf{q}) - a(\mathbf{p}) + a(-\mathbf{q}) + \text{H.c.}] \\ &- \frac{1}{M_0} \int d^3k [a(\mathbf{k})\beta(k)^*\mathbf{k}\cdot\mathbf{P}e^{i\mathbf{k}\cdot\mathbf{Q}} + \text{H.c.}] \\ &- \frac{1}{2}g^2 \int d^3k \frac{|\rho(k)|^2}{\omega(k)\Omega(k)}. \quad (22) \end{aligned}$$

The operator part of this new Hamiltonian has been shown to be the correct generator of time translations in the point-source limit¹⁴ and to have convergent self-energy contributions to any order in perturbation theory.¹⁰

Now that the Hamiltonian is in renormalized form, the dipole approximation

$$\begin{aligned} H &= \frac{1}{2} \int d^3k [\omega(k)^2\phi(\mathbf{k})\phi(-\mathbf{k}) + \pi(\mathbf{k})\pi(-\mathbf{k})] \\ &+ \frac{1}{2M_0} \left[\mathbf{P} - ig \int d^3p \frac{\rho(p)\pi(\mathbf{p})}{\omega(p)\Omega(p)} \right]^2 \\ &- \frac{g^2}{2M_0} \int d^3k \frac{k^2|\rho(k)|^2}{2\omega(k)\Omega(k)} \quad (23) \end{aligned}$$

should no longer give rise to runaway modes. To see that this is indeed the case, the usual procedure is followed.

Mass renormalization is accomplished by decoupling the field and particle operators with the canonical transformation generated by

$$U = \exp \left[-\frac{g}{M_r} \int d^3k \mathbf{k}\cdot\mathbf{P} \frac{\rho^*(k)\phi(\mathbf{k})}{\omega(k)\Omega(k)} \right], \quad (24)$$

where

$$M_r = M_0 \left[1 + \frac{g^2}{3M_0} \int d^3p \frac{p^2}{\omega(p)^2} \frac{|\rho(p)|^2}{\Omega(p)^2} \right]. \quad (25)$$

In the point-source limit [$\omega(k) = k$ for convenience] the renormalized mass is

$$M_r = M_0 [1 + (8/3)\pi g^2] \equiv \lambda^{-1}M_0 \quad (26)$$

and the bare mass is now finite.

¹² E. M. Henley and W. Thirring, *Elementary Quantum Field Theory* (McGraw-Hill Book Co., Inc., New York, 1962), Chap. 11, p. 106.

¹³ K. McVoy and H. Steinwedel, *Nucl. Phys.* **1**, 164 (1956).

¹⁴ E. Nelson, *J. Math. Phys.* **5**, 1190 (1964).

The transformed Hamiltonian is

$$UHU^{-1} = \frac{\mathbf{P}^2}{2M_r} + \frac{1}{2} \int d^3k [\omega(k)^2 \phi(\mathbf{k})\phi(-\mathbf{k}) + \pi(\mathbf{k})\pi(-\mathbf{k})] \\ - \frac{g^2}{2M_0} \left[\int d^3p \mathbf{p} \frac{\rho(p)\pi(\mathbf{p})}{\omega(p)\Omega(p)} \right]^2 \\ - \frac{g^2}{2M_0} \int d^3k \frac{k^2 |\rho(k)|^2}{2\omega(k)\Omega(k)}, \quad (27)$$

where the transformed operators are

$$U\pi(\mathbf{k})U^{-1} = \pi(\mathbf{k}) - \frac{ig}{M_r \omega(k)\Omega(k)} \rho^*(k) \mathbf{k} \cdot \mathbf{P}, \quad (28)$$

$$UQU^{-1} = \mathbf{Q} - \frac{ig}{M_r} \int d^3k \frac{\rho^*(k)\phi(\mathbf{k})}{\omega(k)\Omega(k)} \mathbf{k}. \quad (29)$$

The equation for bound states can now be written down by inspection and is

$$D(k^2) = 1 + \frac{g^2}{3M_0} P \int d^3p \frac{|\rho(p)|^2}{\Omega(p)^2} \frac{p^2}{p^2 - k^2} = 0, \quad (30)$$

or, in terms of the renormalized mass, is

$$1 + \frac{g^2}{3M_0} \omega(k)^2 P \int d^3p \frac{|\rho(p)|^2}{\Omega(p)^2} \frac{p^2}{\omega(p)^2} \frac{1}{p^2 - k^2} = 0. \quad (31)$$

Finally, the runaway modes $\omega(k) = \pm iB$ satisfy the equation

$$1 = \frac{g^2}{3M_r} B^2 \int d^3p \frac{|\rho(p)|^2}{\Omega(p)^2} \frac{p^2}{\omega(p)^2} \frac{1}{\omega(p)^2 + B^2}. \quad (32)$$

In the Appendix it is shown that this equation has no solutions. Thus, there are no runaway modes when the dipole approximation is applied to the renormalized Hamiltonian.

IV. CONCLUSION

It has been conjectured that the runaway modes usually associated with the diagonalization and renormalization of quadratic Hamiltonians, which are the

dipole approximate forms of fully translationally invariant theories, are a result of the misuse of the dipole approximation. An illustration was provided by the polaron Hamiltonian, which was canonically transformed so as to yield a quadratic form in the dipole approximation, and which contained runaway modes upon diagonalization and renormalization. However, it was found that no runaways appeared if the canonical transformation which renormalized the Hamiltonian was applied before the dipole approximation. Thus, the runaway modes which plague nonrelativistic quantum electrodynamics would seem to be avoidable by first finding the canonical transformation which performs the renormalization, i.e., which attaches the self-field to the electron.

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APPENDIX

In order to show that the runaway-mode equation

$$1 = \frac{g^2}{3M_r} B^2 \int d^3p \frac{|\rho(p)|^2}{\Omega(p)^2} \frac{p^2}{\omega(p)^2} \frac{1}{\omega(p)^2 + B^2} \quad (33)$$

has no solutions, compare it with the mass renormalization equation

$$M_r = M_0 + \frac{1}{3} g^2 \int d^3p \frac{|\rho(p)|^2}{\Omega(p)^2} \frac{p^2}{\omega(p)^2}. \quad (34)$$

Upon equating the expressions for M_r , the resulting equation is

$$M_0 = -\frac{1}{3} g^2 \int d^3p \frac{|\rho(p)|^2}{\Omega(p)^2} \frac{p^2}{\omega(p)^2 + B^2}. \quad (35)$$

In the point-source limit this becomes

$$1 = -\frac{16\pi g^2}{3} \lambda M_r \int \frac{dp}{(p + 2\lambda M_r)^2} \frac{p^2}{p^2 + B^2}. \quad (36)$$

Since λ is positive this equation is inconsistent. Thus, there is no solution to the runaway-mode equation for B .