International Journal of Theoretical Physics, Vol. 29, No. 5, 1990

Singular Lagrangian for the Polaron

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Received November 9, 1989

A Lagrangian which describes the electron–phonon interaction is proposed, starting from a simple model of interacting string and charged particle. The Lagrangian is singular, containing both bosonic variables (i.e., phonons) and fermionic ones (i.e., the electron). Symmetry Dirac brackets are used to obtain the BCS Hamiltonian. The addition of a total derivative of a scalar function to the Lagrangian density does *not* alter the quantization procedure.

1. INTRODUCTION

The electron–phonon system (polaron) is basic to the BCS theory of superconductivity for metals (Bardeen *et al.*, 1957). This interaction has been expressed as a Hamiltonian starting from energy considerations (Haken, 1976, Chapter III; Mitra *et al.*, 1987). However, it would be interesting to have a Lagrangian instead, since in this way we can obtain not only the Hamiltonian density, but the remaining conserved quantities. We have found a Lagrangian density by making an analogy with an ideal problem (Haken, 1976, p. 115) of a string on which particles (i.e., electrons) may "walk," these particles being subject to gravity. (We ignore the effect of gravity on the string.) Thus, the combined system represents the interaction of a string, given by a field $q(x, t)$, and a particle described by a second complex field $\psi(x, t)$. The string represents a vibrating lattice of phonons and the particle can be considered as the electron field. Thus, Haken's Lagrangian can be used to describe a polaron (electron plus vibration lattice) if we make the appropriate identification of the variables involved.

However, the Lagrangian density found happens to be linear in the time derivative of the electronic field (i.e., $\sim\dot{\psi}$). As a result, the Lagrangian density is singular, in the sense of Dirac, since we have constraints in phase space between the fields Φ and their canonical momentum densities π_Φ.

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So the canonical variables are not independent of each other and the Dirac (1964) prescription has to be followed to arrive at a sound second quantization scheme. In passing, it is worthwhile mentioning that the Dirac formalism is valid not only for Lagrangians linear in the "velocities" (in our case, $\dot{\psi}$), as can be seen in the recent literature (Galvao and Lemos, 1988; Tapia, 1985).

As said previously, our Lagrangian density has bosonic variables [the field $q(x, t)$] and fermionic variables (the fields ψ, ψ^*). The presence of ψ, ψ^*, which satisfy a Fermi-Dirac type of statistics, forces us to quantize with the help of the symmetric Dirac bracket $\{\cdot, \cdot\}_+^*$ or, simply, the "plus" Dirac bracket (Droz-Vicent, 1966; Franke and Kálnay, 1970; Kálnay and Ruggeri, 1972; Kálnay, 1973) instead of the "minus" Dirac bracket $\{\cdot, \cdot\}_-^*$ (Mukunda and Sudarshan, 1968). The calculation produces the right results in second quantization.

The information contained in the Lagrangian density is richer than that of the Hamiltonian. Along these lines, we have calculated the conserved quantities, evaluating the stress-energy tensor and the angular momentum (Goldstein, 1981, Chapter 12) of the system.

The remainder of this paper is organized as follows. Section 2 states the problem through the writing out of the electron-phonon Lagrangian. Section 3 concentrates on the Dirac procedure to quantize the field variables, arriving at the creation and annihilation operators (i.e., second quantization). Section 4 gives the conclusions and a discussion of the results, mentioning canonical generalizations to our problem.[2]

2. STATEMENT OF THE PROBLEM: THE ELECTRON-PHONON LAGRANGIAN

We will closely follow Haken's arguments (see Figure 1 for definition of the field variables). The procedure to quantize this problem is as follows:

(a) Form the equations of motion.
(b) Form the Lagrangian whose Lagrangian equation will lead back to the equations of motion.
(c) Use the Dirac formalism to find the Hamiltonian and the remaining conserved quantities.
(d) Quantize.
(e) Expand with respect to eigenfunctions in order to obtain the creation and annihilation operators.

We will study steps (a) and (b) in this section, leaving (c)-(e) for Section 3.

[2]For more light on this, see Jánica de la Torre *et al.* (1977). It is natural to include the electromagnetic field in the way described by Chela-Flores *et al.* (1988).

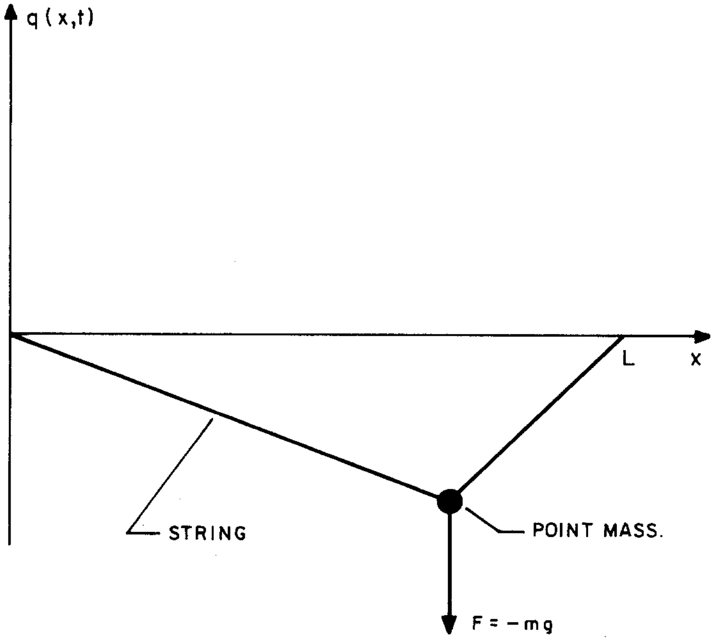

Fig. 1. Interaction between a point mass and a string. The displacement $q(x, t)$ of a string as a function of position x at time t. [Taken from Haken (1976).]

The equations of motion of a vibrating string free from external forces is given by

$$\rho q(x, t) - s\frac{\partial^2 q}{\partial x^2}(x, t) = 0 \tag{1}$$

where ρ is the mass density, q is the transverse displacement at the position x and time t, and s is the tension of the string.

Now the mass m will pull the string down with a force density

$$F = -G\psi^*(x)\psi(x) \tag{2}$$

where $G = mg$, m is the mass of the particle, and g is the acceleration of gravity. In consequence, the equation of motion for the forced vibrating string is

$$\rho q(x, t) - s\frac{\partial^2 q}{\partial x^2}(x, t) = -G\psi^*(x)\psi(x) \tag{3}$$

The interaction between the string and the electron implies that the equations of motion for the electron are

$$i\hbar\dot{\psi}=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+Gq(x,t)\psi(x,t)\right] \tag{4a}$$

$$i\hbar\dot{\psi}^*=\left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-Gq(x,t)\psi^*(x,t)\right] \tag{4b}$$

Equations (3)-(4) are the equations of motion for the fields $q(x, t)$ and $\psi(x, t)$. It is an easy matter to convince oneself that the Lagrangian density which reproduces the equations of motion (3) and (4) is

$$L=\int \mathscr{L}(x)\,dx \tag{5}$$

with $\mathscr{L}$, the Lagrangian density, given by

$$\mathscr{L}(x)=\psi^*(x,t)\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}+\frac{\partial^2}{\partial x^2}\right)\psi(x,t)$$
$$+\frac{1}{2}\left[\rho(\dot{q}(x,t)^2)-s\left(\frac{\partial q}{\partial x}(x,t)^2\right)\right]-Gq(x,t)\psi^*(x,t)\psi(x,t) \tag{6}$$

We will show later that G is related to the electron-phonon coupling constant γ. We can immediately see that the Lagrangian density [equation (6)] is linear in the "velocities" $\dot{\psi}$. In consequence, we have a singular Lagrangian to which the Dirac formalism must be applied. This we do in the following section.

3. DIRAC TREATMENT OF THE SINGULAR LAGRANGIAN

From the Lagrangian density we can evaluate the canonical momentum densities associated with the fields. They are

$$\pi_\psi=\frac{\partial\mathscr{L}}{\partial\dot{\psi}}=i\hbar\psi^* \tag{7a}$$

$$\pi_\psi^*=\frac{\partial\mathscr{L}}{\partial\dot{\psi}^*}=0 \tag{7b}$$

$$\pi_q=\frac{\partial\mathscr{L}}{\partial\dot{q}}=\rho\dot{q} \tag{7c}$$

From equations (7a) and (7b), we observe that the ψ's and π's are related (phase space constraints). We do not have a way to obtain the $\dot{\psi}$'s in terms of the π's. The Lagrangian is singular since the determinant of the 3×3

field matrix $\partial^2\mathscr{L}/\partial\phi_A\,\partial\phi_B$ ($A, B = 1, 2, 3$ and $\phi_1 = \psi$, $\phi_2 = \psi^*$, $\phi_3 = q$) is zero. Then, we have two primary constraints:

$$f_I(x) = \pi_\psi - i\hbar\psi^* \approx 0 \tag{8a}$$

$$f_{II}(x) = \pi_\psi^* \approx 0 \tag{8b}$$

where $\approx$ means weak equality (Dirac, 1964).

To find the secondary constraints, we have to use the consistency equations for the primary constraints. They are (Dirac, 1964; Franke and Kálnay, 1970; Kálnay and Ruggeri, 1972; Kálnay, 1973)

$$\{f_A(x), H\}_- + \sum_{B=\mathrm{I}}^{\mathrm{II}} \int d^3x' \{f_A(x), f_B(x')\}_+ U_B(x') \approx 0 \tag{9}$$

with $A = \mathrm{I}, \mathrm{II}$. Doing the algebra, we find

$$i\hbar U_\mathrm{I} = -\frac{\hbar^2}{2m}\nabla^2\psi(x, t) + Gq(x, t)\psi(x, t) \tag{10a}$$

$$i\hbar U_\mathrm{II} = \frac{\hbar^2}{2m}\nabla^2\psi^*(x, t) - Gq(x, t)\psi^*(x, t) \tag{10b}$$

Equations (10a) and (10b) fix the Lagrange multipliers and they do not produce any additional constraints. Equations (10) are equivalent to equations (4). Next, we evaluate the matrix $C_{AB}(x, x')$ given by

$$C^+_{AB}(x, x') = \{f_A(x), f_B(x')\}_+ \tag{11}$$

where $A, B = 1, 2$ and (Franke and Kálnay, 1970)

$$\{f_A(x), f_B(x')\}_+ = \sum_{C=1}^{3} \int d^3x'' \left[\frac{\delta f_A(x)}{\delta\phi_C(x'')}\frac{\delta f_B(x')}{\delta\pi_{\phi_C}(x'')} + A \leftrightarrow B\right] \tag{12}$$

Then, it is an easy matter to obtain

$$C^+_{AB}(x, x') = \begin{pmatrix} 0 & -i\hbar\delta(x - x') \\ -i\hbar\delta(x - x') & 0 \end{pmatrix} \tag{13}$$

Equation (13) tells us that all the constraints are second class, since their symmetric Poisson bracket determinant is different from zero. The inverse of $C^+_{AB}(x, x')$ is given by

$$(C^+_{AB}(x, x'))^{-1} = \begin{pmatrix} 0 & (i/\hbar)\delta(x - x') \\ (i/\hbar)\delta(x - x') & 0 \end{pmatrix} \tag{14}$$

In order to identify the canonical variables of the theory, we must evaluate the symmetric Dirac bracket $\{F, G\}_+^*$, which can be expressed as (Franke and Kálnay, 1970)

$$\{F, G\}_+^* = \{F, G\}_+ - \iint \{F, f_A(x)\}_+ \times [C_{AB}^+(x, x')]^{-1} \{f_B(x'), G\}_+ \, dx \, dx' \tag{15}$$

The algebra produces

$$\{\psi(x), \psi^*(x')\}_+^* = -\frac{i}{\hbar}\delta(x-x') \tag{16a}$$

$$\{\psi^*(x), \psi^*(x')\}_+ = \{\psi(x), \psi(x')\}_+^* = 0 \tag{16b}$$

$$\{q(x), \pi_q(x)\}_-^* = \delta(x-x') \tag{16c}$$

$$\{q(x), q(x')\}_-^* = \{\pi_q(x), \pi_q(x^1)\}_-^* = 0 \tag{16d}$$

Equations (16a) and (16b) are interesting since they tell us that ψ, ψ^* are conjugate canonical variables. To get the quantum mechanical symmetric commutator, we have to assume that (Kálnay and Ruggeri, 1972)

$$[\cdot, \cdot]_\pm = i\hbar\{\cdot, \cdot\}^* \tag{17}$$

Thus, equations (16) give

$$[\hat{\psi}(x), \hat{\psi}^+(x')]_+ = \delta(x-x') \tag{18a}$$

$$[\hat{q}(x), \hat{\pi}_q(x')]_- = i\hbar\delta(x-x') \tag{18b}$$

etc. [equations (16b) and (16d)]. Now that we have the canonical variables of the theory, we can go to second quantization by expanding ψ, ψ^+, and q in terms of plane waves. Thus,

$$\psi(x) = \sum_k a_k \frac{e^{ikx}}{\sqrt{L}} \tag{19a}$$

$$\psi^+(x) = \sum_k a_k^+ \frac{e^{-ikx}}{\sqrt{L}} \tag{19b}$$

$$q(x) = \sum_x \left(\frac{\hbar}{2\rho\omega_{wL}}\right)^{1/2} (e^{iwx} b_w + e^{-iwx} b_w^+) \tag{19c}$$

In Equations (19), a_k, a_k^+ (b_w, b_w^+) are the annihilation and creation operators for electrons (phonons). According to our approach, the a_k and

b_w must satisfy the following relations

$$[a_k, a_{k'}^+]_+ = \delta_{kk'} \tag{20a}$$

$$[a_k, a_{k'}]_+ = [a_k^+, a_{k'}^+]_+ = 0 \tag{20b}$$

$$[b_w, b_{w'}^+]_- = \delta_{ww'} \tag{20c}$$

$$[b_w, b_{w'}]_- = [b_w^+, b_{w'}^+]_- = 0 \tag{20d}$$

By substituting equations (19) into the Hamiltonian operator given by

$$H = \int \hat{\psi}^+(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\hat{\psi}(x)\,dx + \frac{1}{2\rho}\int \pi_q^2(x)\,dx$$
$$+ \frac{s}{2}\int\left(\frac{\partial q(x)}{\partial x}\right)^2 dx + \int G_q(x)\psi^+(x)\psi(x)\,dx \tag{21}$$

and we end up with

$$H = H_{0,el} + H_{0,l} + H_I \tag{22}$$

where $H_{0,el}$ is the Hamiltonian operator for the electron, $H_{0,l}$ is the Hamiltonian operator for the lattice, and H_I is the electron–phonon interaction Hamiltonian operator. Their explicit forms are (Haken, 1976, Chapter III)

$$H_{0,el} = \sum_k \varepsilon_k a_k^+ a_k \tag{23a}$$

$$H_{0,l} = \sum_w \hbar\psi_w(b_w^+ b_w + \tfrac{1}{2}) \tag{23b}$$

$$H_I = \sum_{k,w} (a_k^+ b_w a_{k+w} g_w^* + a_{k+w}^+ a_k b_w^+ g_w) \tag{23c}$$

where

$$\varepsilon_k = \frac{\hbar^2 K^2}{2m} \tag{23d}$$

and g_w is a coupling constant, which has different expressions for polar crystals and for metals (Haken, 1976, Section 29). It is important to realize that we have written the Hamiltonian operator as in equation (21) since we decided to work with the Dirac brackets [equation (15)] and, at this level, the constraints become strong equations (Galvao and Lemos, 1988).

Also, having the Lagrangian, it is a straightforward matter to obtain the remaining conserved quantities. The stress-energy tensor is given by (Goldstein, 1981, Chapter 12)

$$T_{\mu\omega} = \frac{\partial \mathcal{L}}{\partial \nu_{\rho,\nu}}\eta_{\rho,\mu} - \mathcal{L}\delta_{\mu\nu} \tag{24}$$

with $\eta_1 = \psi$, $\nu_2 = \psi^*$, and $\nu_3 = q$. Doing the algebra, we obtain for the energy density (the T_{00} component) the following expression:

$$T_{00} = \tfrac{1}{2}\rho\dot{q}^2 + \frac{\hbar^2}{2m}\nabla\psi^* \cdot \nabla\psi + \frac{s}{2}(\nabla q)^2 + Gq|\psi|^2 \tag{25}$$

Equations (21) and (25) are equivalent. The energy flux density Q_i, momentum density P_i, and the stress density π_{ij} are given, respectively, by

$$Q_i \equiv T_{0i} = -\frac{\hbar^2}{2m}\left(\dot{\psi}\frac{\partial\psi^*}{\partial x_i} + \dot{\psi}^*\frac{\partial\psi}{x_i}\right) - s\dot{q}\frac{\partial q}{\partial x_i} \tag{26a}$$

$$P_i \equiv T_{i0} = i\hbar\dot{\psi}^*\frac{\partial\psi}{\partial x_i} + \rho\dot{q}\frac{\partial q}{\partial x_i} \tag{26b}$$

$$\pi_{ij} \equiv T_{ij} = -\frac{\hbar^2}{2m}\left(\frac{\partial\psi^*}{\partial x_i}\frac{\partial\psi}{\partial x_j} + \frac{\partial\psi^*}{\partial x_j}\frac{\partial\psi}{\partial x_i}\right)$$

$$- s\frac{\partial q}{\partial x_i}\frac{\partial q}{\partial x_i} - \delta_{ij}\mathscr{L} \tag{26c}$$

As $T_{ij} = T_{ji}$ for $i, j = 1, 2, 3$, we can construct the angular momentum density $\mathscr{M}_{ij}$ (the moment of momentum) which is conserved. Thus,

$$\mathscr{M}_{ij} = i\hbar\psi^*\left(x_j\frac{\partial\psi}{\partial x_i} - x_i\frac{\partial\psi}{\partial x_j}\right) + \rho\dot{q}\left(x_j\frac{\partial q}{\partial x_i} - x_i\frac{\partial q}{\partial x_j}\right) \tag{27}$$

4. CONCLUSIONS AND DISCUSSION

We have studied a singular Lagrangian density suitable for describing the electron-phonon interaction. Because our Lagrangian is singular, the Dirac formalism has been applied to it to identify the canonical variables. The use of the Dirac bracket has allowed us to recover the known commutation and/or anticommutation relations. After completing this stage, we go to a second quantization and our claim that the Lagrangian describes the electron-phonon interaction becomes transparent under plane wave expansion (Section 3).

It is important to emphasize that the addition of a total time derivative to our Lagrangian does not produce different results at the quantization level. For example, adding $(-i\hbar/2)(\psi\dot{\psi}^* + \psi\dot{\psi}^*)$ to equation (6) produces all our constraints are second class, i.e., we obtain that $C^*_{AR}(x, x')$ is still given by equation (13). These results are different from those found by Kálnay and Ruggeri (1972) and Kálnay (1973). The main reason they obtained conflicting results at the quantization level is because they did not use Grassmann variables (Senjanovic, 1976; Negele and Orland, 1988, especially Section 1.5) even at the classical level. Tello-Llanos (1984) shows, for the case of boson variables, that Dirac's generalized mechanics is gauge invariant.

The inclusion of the electromagnetic field can be done by requiring that $i\hbar\nabla \to (i\hbar\nabla + e\bar{A}/c)$. Also, we can add the electromagnetic invariant $(1/8\pi)\, F_{\mu\nu}F^{\mu\nu}$, where F is the usual electromagnetic tensor. In this way, for the stationary phase, this contribution becomes $(1/8\pi)(\nabla x\bar{A})^2$, which is invariant under the gauge transformation $\bar{A} \to \bar{A} + 1/c\nabla\Phi$, where Φ is an arbitrary field. Work along these lines is in progress. Needless to say, the electromagnetic field is a boson field (Jánica de la Torre *et al.*, 1977).

ACKNOWLEDGMENTS

Thanks are due to Prof. Alvaro Restuccia for useful lectures and conversations on Grassmann algebra, and to Mr. Enrique Rodriguez-C., a science supporter in Venezuela. Financial support is acknowledged from the Consejo de Desarrollo Científico (CONDES), Zulia University. This work was done with the support of the Departamentos de Electrónica y Física, Universidad Simón Bolívar, Caracas, Venezuela.

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