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Thermodynamically Equivalent Hamiltonian for Some Many-Body Problems*

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A method which allows a rigorous treatment of the statistical mechanics of a superconductor (Bardeen-Cooper-Schrieffer model) is generalized so as to be applicable to a wider class of many-fermion or many-boson systems.

As an illustration, we study a degenerate boson gas, adopting the "pair Hamiltonian" of Girardeau and Arnowitt. We confirm their finding, for this model, that there is a "gap" in the energy spectrum of the lowest excitations.

I. DESCRIPTION OF THE METHOD

In the "reduced Hamiltonian" of the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity, only two types of operators occur, namely, the occupation number and the pair absorption (and emission) operators:

$$a_{k\uparrow}^* a_{k\uparrow} + a_{-k\downarrow}^* a_{-k\downarrow} \equiv b_{k1}, \quad a_{-k\downarrow} a_{k\uparrow} \equiv b_{k2}. \tag{1}$$

A general expression for the BCS Hamiltonian is then

$$H = \sum_{k\lambda} (E_{k\lambda} b_{k\lambda} + E_{k\lambda}^* b_{k\lambda}^*) + V^{-1} \sum_{k\lambda, k'\lambda'} J_{k\lambda, k'\lambda'} b_{k\lambda}^* b_{k'\lambda'}, \tag{2}$$

$$J_{k\lambda, k'\lambda'} = J_{k'\lambda', k\lambda}^*,$$

(here $E_{k2}=0$). More generally, we will admit Hamiltonians of the form (2) where the operators $b_{k\lambda}$ are specified *bilinear* combinations of the a's and a^*'s, not necessarily those of the BCS theory, though subject to certain conditions to be introduced later. We will also allow the a and a^* operators to refer to either fermions or bosons, since our procedure can be described without specifying the commutation relations. An example of a boson gas problem will be discussed in Sec. II.

A method which was previously used[1,2] to set up the statistical mechanics of the BCS model may be generalized to apply to a whole class of systems, with Hamiltonians of the form (2). The most convenient approach is a variational one[2]: Define new operators,

$$B_{k\lambda} = b_{k\lambda} - \eta_{k\lambda}, \tag{3}$$

where $\eta_{k\lambda}(\lambda = 1, 2, \cdots)$ are trial functions (c numbers, not necessarily real[3]), and subtract from the Hamiltonian (2) a "perturbation" defined as

$$H' = V^{-1} \sum_{k\lambda, k'\lambda'} J_{k\lambda, k'\lambda'} B_{k\lambda}^* B_{k'\lambda'}. \tag{4}$$

The remaining "unperturbed" Hamiltonian may be written

$$H^0 = H - H' = U + \sum_{k\lambda} (G_{k\lambda} b_{k\lambda} + G_{k\lambda}^* b_{k\lambda}^*), \tag{5}$$

where

$$U = -V^{-1} \sum_{k\lambda, k'\lambda'} J_{k\lambda, k'\lambda'} \eta_{k\lambda}^* \eta_{k'\lambda'}, \tag{6}$$

$$G_{k\lambda} = E_{k\lambda} + V^{-1} \sum_{k'\lambda'} J_{k'\lambda', k\lambda} \eta_{k'\lambda'}^*. \tag{7}$$

H^0, being bilinear in the operators a and a^*, can be diagonalized in closed form, e.g., by a Bogoliubov transformation, for any given set of functions $\eta_{k\lambda}$. The free energy F^0 of the corresponding canonical ensemble, defined by

$$\mathrm{Tr} \exp\beta(F^0 - H^0) = 1, \tag{8}$$

can now be minimized by choice of the trial functions:

$$\partial F^0 / \partial \eta_{k\lambda} = \partial F^0 / \partial \eta_{k\lambda}^* = 0. \tag{9}$$

Note that F^0 can be written as

$$F^0 = U + F_1(G_{k\lambda}, G_{k\lambda}^*), \tag{10}$$

where U, $G_{k\lambda}$, and $G_{k\lambda}^*$ depend on η according to (6) and (7). It is then easily seen that (9) is satisfied by setting

$$\eta_{k\lambda} = \partial F_1 / \partial G_{k\lambda}. \tag{11}$$

Substituting this back in (7) leads to a set of coupled integral equations[4] for the functions $G_{k\lambda}$, with solutions depending on the given coefficients $E_{k\lambda}$ and $J_{k\lambda, k'\lambda'}$, and on the temperature β^{-1}.

The essential point is, now, to prove that this variational solution is a *rigorous* one, in a certain sense. For this purpose we note first that the thermal average (for the unperturbed system) of $b_{k\lambda}$,

$$\langle b_{k\lambda} \rangle \equiv \mathrm{Tr}[b_{k\lambda} \exp\beta(F^0 - H^0)] = \partial F_1 / \partial G_{k\lambda}, \tag{12}$$

as is readily seen by substituting (10) and (5) into (8) and then differentiating with respect to $G_{k\lambda}$.[5] From (11) and (12) it follows that the thermal averages of the quantities (3), and also of their conjugates, vanish:

$$\langle B_{k\lambda} \rangle = \langle B_{k\lambda}^* \rangle = 0. \tag{13}$$

Having rigorously determined the free energy F^0 of the unperturbed system H^0 [with (6), (7), and (11)], we now investigate how the perturbation H'(4) affects the free energy F of the system $H = H^0 + H'$. We use a

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[1] N. N. Bogoliubov, D. B. Zubarev, Iu. A. Tserkovnikov, Doklady Acad. Nauk. S.S.S.R. **117**, 788 (1957) [translation: Soviet Phys.-Doklady **2**, 535 (1957)].

[2] G. Wentzel, Helv. Phys. Acta **33** (1960).

[3] In reference 2, they were assumed real, but this is not necessary.

[4] Of course, we consider the limit $V \to \infty$ so that $V^{-1} \sum_k$ becomes a k-space integral.

[5] Note: $\partial\, \mathrm{Tr}[(H^0)^n] / \partial G_{k\lambda} = \mathrm{Tr}[b_{k\lambda} n (H^0)^{n-1}]$, even if $b_{k\lambda}$ does not commute with other terms (like $b_{k\lambda'}^*$) in H^0.

well-known version of the perturbation theory in statistical mechanics (like in reference 1) and assume convergence[6] of the series expansion (in powers of H'). Writing down the mth order correction to the partition function, $\mathrm{Tr}\exp[-\beta(H^0+H')]$, with H' given by (4), one meets with expressions of the following type

$$V^{-m}\,\mathrm{Tr}\{\exp(-\beta H^0)\times\prod_{i=1\cdots 2m}[\exp(\beta_i H^0)C_{k_i}\exp(-\beta_i H^0)]\}, \quad (14)$$

where each C_{k_i} stands for one of the operators $B_{k\lambda}$ or $B_{k\lambda}^*$. (The β_i are integration variables.) At this point, we want to assume that the commutation properties of the $b_{k\lambda}^{(*)}$ are such that, when $H^0(5)$ is written as $U+\sum_k H_k$,

$$[H_k,H_{k'}]=0,\quad [H_k,C_{k'}]=0 \quad\text{for}\quad k\neq k'. \quad (15)$$

It is then easily seen that the trace (14) vanishes, on account of (13), if *one* momentum k_i, say k_1, is different from all the other momenta, $k_2\cdots k_{2m}$, occurring in the product. In order to obtain a nonvanishing term, one has to have *m pairs* of *equal* k_i's so that, after multiplying with the appropriate factors $J_{k\lambda,k'\lambda'}$ and then summing over $k_1\cdots k_{2m}$, the sum runs over only *m independent k* vectors. If one then divides by $\mathrm{Tr}\exp(-\beta H^0)$ and finally writes the sums as integrals, the factors V^{-m} and V^m cancel out and the result becomes volume independent.[7] Hence, to all orders in H' (assuming convergence),

$$\lim_{V\to\infty}\frac{\mathrm{Tr}\exp[-\beta(H^0+H')]}{\mathrm{Tr}\exp(-\beta H^0)}=\text{finite},$$

and

$$\lim_{V=\infty}V^{-1}(F-F^0)=0. \quad (16)$$

We conclude that, subject to the assumptions made, *H' does not affect the volume-proportional part of the free energy.* H^0 alone determines the thermodynamics of the system H *accurately;* it can be termed a "thermodynamically equivalent Hamiltonian." Its eigenvalues are easy to calculate.

Incidentally, in taking first derivatives of F^0, like $S=-\partial F^0/\partial T$ or $p=-\partial F^0/\partial V$, considerable simplification results from the fact that the derivatives via the $\eta_{k\lambda}$ give no contributions, on account of (9). Of course, this is no longer so in the second derivatives (specific heat, compressibility).

Finally, we remark that it may be possible to relax the conditions (15) without altering the end result (16). We shall not discuss such possibilities since (15) is valid both in the BCS theory and in the example we are going to study now.

[6] As to the dangers inherent in this assumption, see reference 2.

[7] Here, the possibility should be mentioned that a term involving, for instance, a product $\cdots B_{k\lambda}\cdots B_{k\lambda}^*\cdots$ is actually an infinite sum (like $\sum_{k'}\cdots$) and thereby introduces a new factor V. This must, of course, be forbidden and is indeed, practically, already ruled out by the condition (15) which limits $b_{k\lambda}$ to a *finite* number of terms $\sim a^*a$ or aa. For example, $b_{k\lambda}=\sum_{k'}a_{k'+k}^*a_{k'}$ is not admissible.

II. DEGENERATE BOSON GAS

We consider a gas of spin-less bosons with (weak repulsive) two-body interactions of spherical symmetry

$$H_{\mathrm{int}}=\tfrac{1}{2}V^{-1}\sum v(q)a_k^*a_{k'}^*a_{k'-q}a_{k+q},\qquad v(q)=v(|q|)\ \text{(real)}. \quad (17)$$

At sufficiently low temperatures, like in the free boson case, a major fraction of the N particles will be condensed in the lowest energy state, supposedly with momentum $k=0$, so that the creation and annihilation operators, a_0^* and a_0, may be replaced by the c number $N_0^{\frac{1}{2}}(\gg 1)$. Retaining in (17) only the "largest" terms, namely those quadratic and linear in N_0, one obtains the "Bogoliubov Hamiltonian"[8]:

$$H^{\mathrm{I}}=\tfrac{1}{2}V^{-1}N_0^2v(0)+\sum_k[f_k^{\mathrm{I}}a_k^*a_k+\tfrac{1}{2}h_k^{\mathrm{I}}(a_k^*a_{-k}^*+a_{-k}a_k)], \quad (18)$$

where $k=0$ is *excluded* from the sums, and

$$f_k^{\mathrm{I}}=k^2/2m+V^{-1}N_0[v(k)+v(0)],\qquad h_k^{\mathrm{I}}=V^{-1}N_0v(k). \quad (19)$$

The H^{I} problem is rigorously soluble. The main asset attributed to this theory is the phonon character of the lowest excitations.

However, we want to go one step further, following Girardeau and Arnowitt.[9] One observes that in the ground state of H^{I}, not only the occupation numbers $N_k=a_k^*a_k$, but also the quantities $a_k^*a_{-k}^*$ and $a_{-k}a_k$ have nonvanishing expectation values (they even become large as $k\to 0$). To obtain an improved approximation, one would then, in the first place, want to include the interaction terms which are quadratic in these operators:

$$H=H^{\mathrm{I}}+\tfrac{1}{2}\sum_{kk'}[i_{kk'}^{\mathrm{I}}(a_k^*a_k)(a_{k'}^*a_{k'})+j_{kk'}^{\mathrm{I}}(a_k^*a_{-k}^*)(a_{-k'}a_{k'})], \quad (20)$$

$$i_{kk'}^{\mathrm{I}}=V^{-1}[v(k-k')+v(0)],\qquad j_{kk'}^{\mathrm{I}}=V^{-1}v(k-k'). \quad (21)$$

This H is what Girardeau and Arnowitt[9] call "pair Hamiltonian." They use a variational method, in conjunction with a Bogoliubov transformation, to analyze this problem, and they find that a "gap" appears in the spectrum of excitations.

Our treatment of this problem will be more general in that we allow thermal excitation. Then, the parameter N_0 in (18), (19) will become temperature dependent, and it should finally be identified with the thermal average of the operator

$$N_0=N-\sum_k a_k^*a_k, \quad (22)$$

[8] N. N. Bogoliubov, J. Phys. (U.S.S.R.) **11**, 23 (1947). In the terms $k\neq 0$, one should, strictly speaking, introduce the number-conserving operators $a_k^*a_0N_0^{-\frac{1}{2}}$ and $N_0^{-\frac{1}{2}}a_0^*a_k$, but these we may safely re-name a_k^* and a_k, without changing anything essential.

[9] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959).

($k=0$ is again excluded from the sum) where N is the given total number of particles.[10] An alternative procedure[11] is to substitute for N_0, in $H^{\rm I}$, the *operator* (22). This is the course we shall follow because it fits well with our treatment of the i, j terms in (20).

With the substitution (22) made in (18) and (19), the Hamiltonian (20) becomes

$$H=\sum_k\left[f_k^{\rm II}a_k^*a_k+\tfrac{1}{2}h_k^{\rm II}(a_k^*a_{-k}^*+a_{-k}a_k)\right]+\tfrac{1}{2}\sum_{kk'}\left[i_{kk'}(a_k^*a_k)(a_{k'}^*a_{k'})+j_{kk'}(a_k^*a_{-k}^*)\times(a_{-k'}a_{k'})+l_{kk'}(a_k^*a_{-k}^*+a_{-k}a_k)(a_{k'}^*a_{k'})\right]+\tfrac{1}{2}V^{-1}N^2v(0), \quad (23)$$

with the following meaning of the coefficients:

$$\begin{aligned}&f_k^{\rm II}=k^2/2m+V^{-1}Nv(k), \quad h_k^{\rm II}=V^{-1}Nv(k),\\ &i_{kk'}=V^{-1}[v(k-k')-v(k)-v(k')],\\ &j_{kk'}=V^{-1}v(k-k'), \quad l_{kk'}=-V^{-1}v(k).\end{aligned} \quad (24)$$

Now, H (apart from the additive constant, and after some relabeling in the $l_{kk'}$ terms[12]) has the form (2) if we identify

$$b_{k1}=a_k^*a_k, \quad b_{k2}=a_{-k}a_k. \quad (25)$$

Introducing the trial functions

$$\eta_{k1}=\xi_k, \quad \eta_{k2}=\eta_k, \quad (26)$$

which we may take *real* without losing generality, we can immediately write down H^0, as given by (5), (6), (7):

$$H^0\equiv H-H'=U+\sum_k\left[f_ka_k^*a_k+\tfrac{1}{2}h_k(a_k^*a_{-k}^*+a_{-k}a_k)\right], \quad (27)$$

where

$$U=-\tfrac{1}{2}\sum_{kk'}\left[i_{kk'}\xi_k\xi_{k'}+j_{kk'}\eta_k\eta_{k'}+2l_{kk'}\eta_k\xi_{k'}\right]+\tfrac{1}{2}V^{-1}N^2v(0), \quad (28)$$

$$\begin{aligned}f_k&=f_k^{\rm II}+\sum_{k'}(i_{kk'}\xi_{k'}+l_{k'k}\eta_{k'}),\\ h_k&=h_k^{\rm II}+\sum_{k'}(l_{kk'}\xi_{k'}+j_{kk'}\eta_{k'}).\end{aligned} \quad (29)$$

As is well known, the diagonalization of H^0 is achieved by the transformation[8]

$$a_k=u_k\alpha_k+v_k\alpha_{-k}^*, \quad (30)$$

with

$$u_k^2=\tfrac{1}{2}[1+(f_k/\epsilon_k)], \quad v_k^2=\tfrac{1}{2}[-1+(f_k/\epsilon_k)], \quad (31)$$

$$\epsilon_k=(f_k^2-h_k^2)^{\frac{1}{2}}, \quad (32)$$

(assuming $|f_k|\geqslant|h_k|$), with the result

$$H^0=E^0+\sum_k\epsilon_kn_k, \quad n_k=\alpha_k^*\alpha_k(=0,1,2,\cdots), \quad (33)$$

$$E^0=U+\tfrac{1}{2}\sum_k(\epsilon_k-f_k). \quad (34)$$

The free energy of the corresponding canonical ensemble is

$$F^0=E^0+F_2, \quad (35)$$

$$\begin{aligned}F_2&=-\beta^{-1}\sum_k\ln\sum_{n_k}\exp(-\beta\epsilon_kn_k)\\&=\beta^{-1}\sum_k\ln[1-\exp(-\beta\epsilon_k)].\end{aligned} \quad (36)$$

We note

$$\begin{aligned}\langle n_k\rangle&\equiv{\rm Tr}[n_k\exp\beta(F^0-H^0)]\\&=\partial F_2/\partial\epsilon_k=(\exp\beta\epsilon_k-1)^{-1}.\end{aligned} \quad (37)$$

Also, by use of (30) and (31):

$$\begin{aligned}\langle a_k^*a_k\rangle&=u_k^2\langle n_k\rangle+v_k^2\langle n_k+1\rangle=(f_k/\epsilon_k)(\langle n_k\rangle+\tfrac{1}{2})-\tfrac{1}{2},\\ \langle a_{-k}a_k\rangle&=u_kv_k\langle 2n_k+1\rangle=-(h_k/\epsilon_k)(\langle n_k\rangle+\tfrac{1}{2}).\end{aligned} \quad (38)$$

It remains to find the trial functions (26) which minimize F^0:

$$\partial F^0/\partial\eta_{k\lambda}=\partial E^0/\partial\eta_{k\lambda}+\sum_{k'}\langle n_{k'}\rangle\partial\epsilon_{k'}/\partial\eta_{k\lambda}=0 \quad (39)$$

[see (35) and (37)]. Note that $\epsilon_{k'}$ (32) depends on ξ and η through f and h (29). The solution of (39) can be anticipated from (3), (13) and (38), and is indeed

$$\begin{aligned}\xi_k&=\langle a_k^*a_k\rangle=(f_k/\epsilon_k)(\langle n_k\rangle+\tfrac{1}{2})-\tfrac{1}{2},\\ \eta_k&=\langle a_{-k}a_k\rangle=-(h_k/\epsilon_k)(\langle n_k\rangle+\tfrac{1}{2}).\end{aligned} \quad (40)$$

This, together with (27), (28), (29), determines the "thermodynamically equivalent Hamiltonian." Its diagonal representation (33) makes it obvious that the conditions (15) are satisfied, and we can trust F^0 to describe the thermodynamics of the system without any error.

Substitution of (40) into (29) furnishes two coupled integral equations for f_k and h_k, nonlinear because of (32). Contrary to the case of superconductivity (where the terms corresponding to $h_k^{\rm II}$ and $l_{kk'}$ in (29) are zero), there is no "trivial solution" ($h_k=0$, $\eta_k=0$), and an expansion in powers of i, j, and l may be possible, depending on the density $V^{-1}N$ and the properties of the function $v(k)$. All admissible solutions are subject to the conditions $|f_k|\geqslant|h_k|$ (for all k) and $\langle N_0\rangle\gg 1$ where

$$\langle N_0\rangle=N-\sum_k\xi_k. \quad (41)$$

For the case of zero temperature ($\langle n_k\rangle=0$), we have verified that our method is equivalent to the variational Ansatz of Girardeau and Arnowitt.[9] On the other hand, if one wants to study the thermodynamic properties of the system, it is important to note that the coefficients f_k and h_k, as given by (29) and (40), now depend on the temperature through $\langle n_k\rangle$ (37). This is the same situation as in the theory of superconductivity where the spectrum of elementary excitations (the gap) appears as temperature dependent, in the equivalent Hamiltonian. Since the condition $\langle N_0\rangle\gg 1$ precludes a study of the

[10] For the Hamiltonian $H^{\rm I}(i^{\rm I}, j^{\rm I}=0)$, this determination of N_0 is carried through with great care, by means of a grand ensemble, in a recent paper by A. E. Glassgold, A. N. Kaufman, and K. M. Watson, UCRL-9149 University of California Radiation Laboratory Report (unpublished). Since their results afford an opportunity to check our method we shall come back to the $H^{\rm I}$ problem in the Appendix.

[11] See, e.g., K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117 (1957).

[12] Re-ordering of factors leaves the V-proportional part unchanged.

phase transition ($\langle N_0\rangle/N \to 0$), we shall not here discuss such matters in detail.

In conclusion, we add some remarks on the low-momentum excitations. As was mentioned already, Girardeau and Arnowitt[9] have found that, for their model, the phonon law ($\epsilon_k/k \to \text{const}\neq 0$, as $k\to 0$) is invalid. This statement is important enough as to merit special consideration. From (24), (29), and (41), one finds easily

$$\begin{aligned}\lim_{k\to 0} f_k &= V^{-1}\langle N_0\rangle v(0) - V^{-1}\textstyle\sum_{k'} v(k')\eta_{k'},\\ \lim_{k\to 0} h_k &= V^{-1}\langle N_0\rangle v(0) + V^{-1}\textstyle\sum_{k'} v(k')\eta_{k'}.\end{aligned} \tag{42}$$

Unless one of the two terms on the right-hand sides in (42) vanishes, ϵ_k (32) *cannot tend to zero.* Now $v(0)$, or the space integral over the two-body potential, can hardly vanish, and would presumably be positive. For an estimate of the other term, we use (40) with $\langle n_k\rangle = 0$ (zero temperature) and $h_k \approx h_k^{\mathrm{II}}$ (24):

$$-V^{-1}\textstyle\sum_k v(k)\eta_k \approx \frac{1}{2}(V^{-1}N)V^{-1}\sum_k [v(k)]^2/\epsilon_k. \tag{43}$$

This expression is certainly >0 (note that, then, $|f_k|>|h_k|$ for $k\to 0$, as is desired for consistency). A cancellation of the term (43) owing to the terms $\sim\xi, \eta$ in (29) cannot be expected although this might possibly happen under very special circumstances. We therefore arrive at the same conclusion as Girardeau and Arnowitt:

$$\lim_{k\to 0}\epsilon_k > 0, \tag{44}$$

for the system described by the Hamiltonian (20). Their value for the energy gap agrees with (42) at zero temperature.

It is a different question whether other interaction matrix elements in (17) which we have deliberately omitted in (20) can cause the energy gap to vanish, independently of the density (and temperature). With a perturbation treatment, for the case of weak interactions, the necessary cancellations appear highly unlikely, in view of the incongruity of the various energy denominators coming in, but a convincing proof is difficult.[13]

It would be daring to extrapolate our results to the case of *strong* interactions or to real liquid helium where, even if inconsistencies were avoidable, the meaning of an analysis in terms of single particle states would be far from clear, to say the least. More convincing are then Feynman's[14] qualitative arguments concerning the structure of the wave functions in configuration space, from which the phonon law (for small k) appears to follow.

APPENDIX: THE H^{I} PROBLEM

Our method can readily be applied to the system characterized by the Hamiltonian (18), just by changing the meaning of the i, j coefficients:

$$\begin{aligned} i_{kk'}{}^{\mathrm{I}} &= 0, \quad i_{kk'} = V^{-1}[-v(0)-v(k)-v(k')],\\ j_{kk'}{}^{\mathrm{I}} &= 0, \quad j_{kk'} = 0.\end{aligned} \tag{45}$$

The i and l terms in (23) have their origins now exclusively in the substitution (22), and one should then expect agreement with such calculations as those by Glassgold, Kaufman, and Watson, who determine $N_0 \equiv \langle N_0\rangle$ by other considerations.[10] Indeed, their values for f_k and h_k agree completely with those obtained by substituting (45) in our Eqs. (29), etc., and also the ground-state energies agree. This finding is not altogether trivial because we have assumed convergence in the perturbation treatment of H' (4), and the agreement may be regarded as an indirect confirmation of this convergence, at least in the case (45).

Incidentally, even in this case ϵ_k does not strictly tend to zero as $k\to 0$. Indeed,

$$\lim_{k\to 0}(f_k - h_k) = -\Delta\mu(>0),$$

where $\Delta\mu$ is defined in the paper quoted in reference 10, Eqs. (3.11) and (3.12). Only if $\Delta\mu$ is neglected does the phonon law result. Of course, we regard H^{I} as an even less realistic Hamiltonian than our H (20).

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[13] This would not exclude the possible existence of a phonon spectrum extending through the gap, for there may be eigenstates of the complete Hamiltonian which are not even approximately eigenstates of the pair Hamiltonian (20). Such a situation might be compatible with the conclusions derived by N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).

[14] R. P. Feynman, Phys. Rev. **94**, 262 (1954).