Nonlinear Schrödinger equation: A testing ground for the quantization of nonlinear waves*

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Quantization of the nonlinear Schrödinger equation is carried out by the method due to Kerman and Klein. A viable procedure is inferred from the quantum interpretation of the classical (soliton) solution. The groundstate energy for a system with n particles is calculated to an accuracy which includes the first quantum correction to the semiclassical result. It is demonstrated that the exact answer can be obtained systematically only at the next level of approximation. For the calculation of the first quantum correction, the quantum theory of the stability of periodic orbits in field theory is developed and discussed. Since one is dealing with a finite many-body problem, the field theory can be written so that no infinite terms are encountered, but the Hamiltonian can also be artificially rearranged so as to destory this feature. For learning purposes the calculations are carried out with the various alternatives, and our methods prove capable of providing a uniform final result.

I. INTRODUCTION

This is the second in a sequence of papers whose aim is the development and exposition of a nonperturbative, completely quantum-mechanical approach to selected problems in the quantization of nonlinear field theories. This method, first developed for problems of collective motion in the many-body problem,¹ was introduced into the present context by Goldstone and Jackiw² to treat the problem of "quantization about a static solution of the classical nonlinear field equations." Our previous paper involved directly an extension of this latter work.^{3,4}

The present paper has two objectives. The first is to show that the same general method is readily applicable to instances where the known classical solution is periodic in time and nondissipative, i.e., the energy is finite and time-independent. Such solutions are the analogs of bound orbits in particle mechanics, and as has clearly been shown,⁵ each gives rise upon quantization to a spectrum of bound states. The second aim of the present work is to show (by example) that problems of renormalization of infinities and higherorder effects can be handled quite consistently with the present method. In the previous treatments,^{5,6} this involved the classical theory of stability of periodic orbits. In this work, we present the analogous quantum theory, leaning in no way on the classical analysis.

To achieve these aims, we have chosen an exactly soluble, completely finite, nonrelativistic field theory^{7,8}: nonrelativistic bosons of mass *m* interacting in pairs via an attractive δ -function potential, in one space dimension. The theory in question is defined by the Hamiltonian

.

$$H = \frac{\hbar^2}{2m} \int dx \, \frac{d}{dx} \, \psi^{\dagger}(x) \, \frac{d}{dx} \, \psi(x)$$
$$- \frac{1}{2} K \int dx \, \psi^{\dagger}(x) \, \psi^{\dagger}(x) \, \psi(x) \, \psi(x) \quad (1.1)$$

[where $\psi(x)$ is *purely* a destruction operator] and by the commutation relations

$$[\psi(x), \psi^{\dagger}(y)] = \delta(x - y) .$$
 (1.2)

The theory defined by (1.1) and (1.2) is completely finite and possesses for each value of n. where n is the number of particles and is the value of the constant of the motion,

$$\int \psi^{\dagger}(x) \,\psi(x) \equiv \hat{N} \,, \qquad (1.3)$$

just one bound state, with energy

$$E_n = -\frac{1}{24} \left(\frac{K^2 m}{\hbar^2} \right) (n^3 - n) .$$
 (1.4)

In addition, all possible scattering amplitudes are known.7

As we come to understand from our method, the "structure" of (1.4) is to be understood as follows: $(K^2 m/\hbar^2)$ is the only energy unit in the problem. A semiclassical approximation then yields the n^3 term only. Relative to this leading term the quantum corrections generate a series in reciprocal powers of n. Thus the first quantum correction vanishes, as we shall rederive repeatedly (for learning purposes). The second quantum correction is needed to derive the second term of (1.4). Since neither we nor previous authors⁸ has so far made this calculation, any

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implication in previous work that this term has been derived from a field theory is in our opinion slightly misleading. However, the methods developed here can certainly be applied to this problem. (Of course, we can include this term by *requiring* that we obtain the known answer for n=1, as has been done in the previous work.)

The outline of this paper is as follows. We deal in principle only with the bound-state problem, though the calculation of quantum corrections brings in successively more complicated scattering states as we go to higher order. In Secs. II-V, we develop a method of attacking the bound-state problem depending only on (1.1)-(1.3) and the "field equation" which follows from (1.1) and (1.2), namely ($\hbar = m = 1$ henceforth)

$$i\dot{\psi}(x) = [\psi(x), H]$$

= $-\frac{1}{2} \frac{d^2}{dx^2} \psi(x) - K\psi^{\dagger}(x) \psi(x) \psi(x)$, (1.5)

which has only finite matrix elements. In developing the solution both the translational and Galilean invariance of H play a role.

By formal commutation (1.1) becomes

$$H = \frac{1}{2} \int \frac{d}{dx} \psi^{\dagger}(x) \frac{d}{dx} \psi(x)$$
$$- \frac{1}{2} K \int dx \psi^{\dagger}(x) \psi(x) \psi^{\dagger}(x) \psi(x)$$
$$+ \frac{1}{2} K \delta(0) \int dx \psi^{\dagger}(x) \psi(x) . \qquad (1.6)$$

When treated in this form the problem has the essential features of relativistic one-dimensional field theories requiring simple renormalizations. In Secs. VI and VII we show that we have or can develop the tools to deal with this problem. It requires, in effect, that we understand fully the quantum field theory of small oscillations about bound spectra. Some of the more mathematical details of the theory are treated in Appendix B.

In Appendix A, we treat a point which is essential for future developments. In the present work, we appear to lean heavily on the number quantization condition following from (1.3). This is not available for neutral theories. We therefore show in Appendix A that the enforcement of the property of Galilean invariance yields equivalent information.

II. SEMICLASSICAL QUANTIZATION

Consider (1.5) as a classical partial differential equation

$$i\psi(x, t) = -\frac{1}{2} \frac{d^2}{dx^2} \psi(x, t) - K\psi^{\dagger}(x, t) \psi(x, t) \psi(x, t) \cdot (2.1)$$

A known solution⁹ is

$$\psi^{(c)}(x,t) = (2/K)^{1/2} \frac{|\omega|^{1/2} e^{i\omega t}}{\cosh(2|\omega|)^{1/2} x}, \qquad (2.2)$$

with energy

$$E^{(c)} = H(\psi^{(c)}) = -(2\sqrt{2}/3K) |\omega|^{3/2} . \qquad (2.3)$$

This can be calculated directly or through the intermediary of a simple virial theorem obtainable from (2.1) after removal of the time dependence, namely

$$0 = \int dx \left[\omega | \psi^{(c)} |^2 - \frac{1}{2} \left| \frac{d}{dx} \psi^{(c)} \right|^2 - \frac{1}{2} K (|\psi^{(c)}|^2)^2 \right].$$
(2.4)

When added to the functional $H(\psi^{(c)})$, we have that

$$E^{(c)} = \int dx \left(\left| \frac{d}{dx} \psi^{(c)} \right|^2 - \omega |\psi^{(c)}|^2 \right)$$
(2.5)

Equation (2.3) can be used directly in a variant of the Wilson-Sommerfeld quantization condition, namely

$$n = \int_{0}^{E_{n}} \frac{d\epsilon}{|\omega(\epsilon)|}$$
(2.6)

[which follows from the correspondence equation $\omega = (dE/dn)$]. We thus find

$$E_n = -\frac{1}{24}K^2 n^3 , \qquad (2.7)$$

$$\omega_n = (dE_n/dn) = -\frac{1}{8}K^2 n^2 . \qquad (2.8)$$

The same result is obtained by substituting the number quantization condition

$$\int dx \, |\psi^{(c)}|^2 = 2 \, (2 \, |\omega|)^{1/2} / K = n \tag{2.9}$$

in (2.3). Inserting the relation (2.8) into (2.2) shows that the latter represents a class of solutions (t=0)

$$\psi_n^{(c)}(x) = \frac{1}{2} \frac{K^{1/2} n}{\cosh(\frac{1}{2}Knx)} \quad . \tag{2.10}$$

As developed in the next section, the physical interpretation of (2.10) is the basis for our quantum approach.

III. CLASSICAL RESULT AS LIMIT OF A QUANTUM THEORY

Since the correspondence principle tells us that $\omega_n \cong E_n - E_{n-1}$ [Eq. (2.8)], the quantum interpretation of $\psi_n^{(c)}$, Eq. (2.10), is, in fact, obvious, namely (up to terms of relative order n^{-1})

$$\psi_n^{(c)}(x) \cong \langle n-1 | \psi(x) | n \rangle \equiv \psi_n(x) .$$
(3.1)

In this interpretation $|n\rangle$ is the ground state for *n* bosons, and we are neglecting center-of-mass motion or recoil, thus taking the kinetic mass of the states $|n\rangle$, $|n-1\rangle$,... to be infinite. This approximation will simplify the treatment of this section and the next. Here we shall lean on a result which is not obvious, but will be proved in Sec. V: To the first *two* orders in the energy, namely $O(n^3)$ and $O(n^2)$, this "fixed source" approach is valid, provided that in the Hamiltonian (and consequently in the equations of motion) we replace *m* by an "enhanced" mass m_n .

$$m_n = m[n/(n-1)] \to n/(n-1)$$
. (3.2)

The quantum method is based on the following assumptions: (i) The matrix elements (3.1) are the dominant elements in the theory for large n. (ii) The classical field equation should be the

limit of a suitable matrix element of the quantum field equation.

More carefully now we define

$$\omega_n = E_n - E_{n-1} , \qquad (3.3)$$

where

$$H|n\rangle = E_n|n\rangle \quad . \tag{3.4}$$

From (1.5) and (3.1), we find

$$\omega_n \psi_n(x) = -\frac{1}{2m_n} \frac{d^2}{dx^2} \psi_n(x)$$
$$-K \langle n-1 | \psi^{\dagger}(x) \psi(x) \psi(x) | n \rangle . \qquad (3.5)$$

The desire to reach the classical equation suggests a treelike approximation,

$$\langle n-1 | \psi^{\dagger}(x) \psi(x) \psi(x) | n \rangle \cong \langle n-1 | \psi^{\dagger}(x) | n-2 \rangle \langle n-2 | \psi(x) | n-1 \rangle \langle n-1 | \psi(x) | n \rangle$$

$$= | \psi_{n-1}(x) |^{2} \psi_{n}(x)$$

$$= | \psi_{n}(x) |^{2} \psi_{n}(x) \left[1 + O\left(\frac{1}{n}\right) \right].$$

$$(3.6)$$

Thus (3.5) becomes

$$\omega_n \psi_n(x) = -\frac{1}{2m_n} \frac{d^2}{dx^2} \psi_n(x) - K |\psi_n(x)|^2 \psi_n(x) , \qquad (3.7)$$

which is the classical equation, to leading order. In the same approximation

$$\left\langle n \left| \int dx \, \psi^{\dagger}(x) \, \psi(x) \right| \, n \right\rangle = \int dx \, |\psi_n(x)|^2 = n \, . \tag{3.8}$$

The combination of (3.7) and (3.8) implies (3.1), our starting point.

Next, using the same approximation as in (3.6) we calculate the energy and find

$$E_{n} = \langle n | H | n \rangle$$

$$= \frac{1}{2m_{n}} \int dx \left| \frac{d}{dx} \psi_{n}(x) \right|^{2} - \frac{1}{2}K \int |\psi_{n}(x)|^{2} |\psi_{n-1}(x)|^{2} \cong E^{(c)}(n, m_{n}) + \frac{1}{2} \frac{d}{dn} \left\{ \frac{1}{2}K \int [|\psi_{n}(x)|^{2}]^{2} \right\}$$

$$= -\frac{1}{24}K^{2}n^{3} [n/(n-1)] + \frac{1}{8}K^{2}n^{2} \cong E^{(c)} + \frac{1}{12}K^{2}n^{2} , \qquad (3.9)$$

in which we have consistently kept only the first two orders of n.

The correct coefficient of n^2 is known to be zero.^{7,8} The calculation in (3.9), as will be clarified in Sec. V, includes the effect of recoil and of *n* fluctuation. What is missing to this order is the effect of virtual dissociation of the bound state $|n\rangle$ into $|n-1\rangle$ and a single particle (called oneloop effects in field theory and ground-state correlations in the many-body problem). These are studied in the next section.

IV. THE ONE-LOOP QUANTUM CORRECTION

In contrast to relativistic field theories, the effects considered here are finite at all stages of calculation. They take into account the fact that the state $\psi(x)|n\rangle$ has nonvanishing overlap with states other than $|n-1\rangle$. We must then weigh the relative overlaps with various states of n-1 particles such as $|n-2,k\rangle$, $|n-3,k_1,k_2\rangle$, $|n-3,2(k)\rangle,\ldots$. Here $|n-2,k\rangle$ is a scattering state (with suitable boundary conditions) containing asymptotically one free boson, momentum k, and the bound state $|n-2\rangle$; $|n-3,k_1,k_2\rangle$ is asymptotically a three-particle state; $|n-3,2(k)\rangle$ is asymptotically a two-particle state consisting of a heavy and a light bound state. In this classification, only the kinetic energy of the light particles is taken into account, though this approximation must be rectified if the next quantum correction is sought.

To sort out the different orders (in n^{-1}) of the quantum theory, an assumption which proves to be self-consistent is that

$$\langle n-2, k | \psi(x) | n \rangle \sim \langle n-1 | \psi(x) | n-1, k \rangle \sim n^{-1/2} \langle n-1 | \psi(x) | n \rangle,$$

$$(4.1)$$

$$\langle n-3, k_1, k_2 | \psi(x) | n \rangle \sim \langle n-1, k | \psi | n, k' \rangle_{\text{connected}} \sim \langle n-3, 2(k) | \psi(x) | n \rangle \sim n^{-1} \langle n-1 | \psi(x) | n \rangle , \qquad (4.2)$$

with an obvious extension to more complex amplitudes if (4.1) and (4.2) are correct. The *n* dependence in (4.1) and (4.2) was guessed by comparing the energy correction derived below with the discussion following (1.4), but only the existence of a suitable hierarchy of magnitudes need be assumed in order to proceed.

To calculate the $O(n^2)$ terms in E_n , we require only the amplitudes in (4.1). We thus define

$$\chi_k(x) \equiv \langle n-1 | \psi(x) | n-1, k \rangle , \qquad (4.3)$$

$$\eta_k(x) \equiv \langle n-2, k | \psi(x) | n \rangle \quad . \tag{4.4}$$

where the n dependence of these amplitudes and the scattering state boundary conditions are both understood.

If our estimate (4.1) and (4.2) is correct, then Eq. (3.9) for the energy has to be augmented by terms at most quadratic in the amplitudes (4.3)and (4.4). As a typical contribution we have

$$\langle n | \psi^{\dagger}(x) \psi^{\dagger}(x) \psi(x) \psi(x) | n \rangle =$$
 "classical" term

+
$$\sum_{k',k'',k'''} \langle n | \psi^{\dagger}(x) | n - 2, k' \rangle \langle n - 2, k' | \psi^{\dagger}(x) | n - 3, k'' \rangle$$

 $\times \langle n - 3, k'' | \psi(x) | n - 2, k''' \rangle \langle n - 2, k''' | \psi(x) | n \rangle + \cdots$ (4.5)

We write consistently

$$\langle n-2, k' | \psi^{\dagger}(x) | n-3, k'' \rangle = \delta_{k',k''} \langle n-2 | \psi^{\dagger}(x) | n-3 \rangle [1+O(n^{-1})] .$$
(4.6)

This reduces the explicit term in (4.5) to

$$\sum_{k} |\psi_{n}(x)|^{2} |\eta_{k}(x)|^{2} , \qquad (4.7)$$

ignoring n fluctuations in this already corrective term. In addition to terms such as (4.7), there occurs as part of (4.5) a term of the form

$$\sum_{k} \langle n | \psi^{\dagger}(x) | n-1 \rangle \langle n-1 | \psi^{\dagger}(x) | n-2 \rangle \langle n-2 | \psi(x) | n-2, k \rangle \langle n-2, k | \psi(x) | n \rangle \cong \psi_{n}^{2}(x) \chi_{k}(x) \eta_{k}(x) .$$

$$(4.8)$$

For low-order calculations enumeration of the various contributions is quite straightforward. For higherorder effects the development of an algorithm would be helpful.

The method of analysis having been exemplified, we next quote the expression for E_n calculated by this means and certified correct to the first two orders in n, namely ($\psi \equiv \psi_n$)

$$E_{n} = -\frac{1}{2m_{n}} \int dx \left[\frac{d}{dx} \psi(x) \right]^{2} - \frac{1}{2}K \int dx \psi^{4}(x) + \frac{1}{2} \frac{d}{dn} \left[\frac{1}{2}K \int dx \psi^{4}(x) \right] - \omega_{n} \sum_{k} \int dx |\eta_{k}(x)|^{2} + \frac{1}{2m} \sum_{k} \int dx \left| \frac{d}{dx} \eta_{k}(x) \right|^{2} - 2K \sum_{k} \int dx \psi^{2}(x) |\eta_{k}(x)|^{2} - \frac{1}{2}K \sum_{k} \int dx \psi^{2}(x) (\eta_{k} \chi_{k} + \eta_{k}^{*} \chi_{k}^{*}) .$$
(4.9)

The presence of the first of the one-loop terms in (4.9) requires additional explanation. The equation for $\psi_n(x)$ itself is modified by the quantum fluctuations, and we must ask if the corresponding change in ψ_n will affect the energy to the order considered. This is investigated by replacing $\psi_n - \psi_n + \delta \psi$ in (3.9) and examining terms linear in $\delta \psi$. Utilizing the classical equation (3.7), we find easily the additional terms $\omega_n \delta(\int dx \psi_n^2)$. This is not zero, since we have a change in the normal-

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ization condition to this order

$$n = \left\langle n \left| \int dx \psi^{\dagger}(x) \psi(x) \right| n \right\rangle$$

= $\int dx \psi_n^2(x) + \sum_k \int dx |\eta_k(x)|^2$,
 $\delta \int dx \psi_n^2 = -\sum_k \int dx |\eta_k(x)|^2$. (4.10)

We have now accounted fully for the expression (4.9).

We have thus reduced the problem to the computation of the matrix elements [(2.3) and (2.4)], χ_k and η_k . We show that to the required order, these satisfy linear coupled differential equations defining a quantum scattering problem which is the quantum analog of the classical theory of stability of periodic orbits against small perturbations. However, nothing is gained for our purposes by pursuing this analogy.

The equations for χ_k and η_k^* (it is these functions which are coupled) are derived from (1.5) by the arguments illustrated sufficiently in this section, insisting only that terms linear in these amplitudes be retained. The resulting equations, remembering also that

$$H|n,k\rangle = [E_n + (k^2/2)]|n,k\rangle,$$
 (4.11)

are

Omitted terms are at least of relative order $[|\eta|^2/|\psi|^2] \sim n^{-1}$.

 $[2\omega_n - (k^2/2)]\eta_k^*(x) = -\frac{1}{2}\frac{d^2}{dx^2}\eta_k^*(x) - K[2\psi^2(x)\eta_k^*(x) + \psi^2(x)\chi_k(x)].$

 $(k^2/2)\chi_k(x) = -\frac{1}{2}\frac{d^2}{dx^2}\chi_k(x) - K[2\psi^2(x)\chi_k(x) + \psi^2(x)\eta_k^*(x)],$

Before solving these equations, let us note that they can be used to simplify the energy (4.9). Here we need only the second of the integrated forms of (4.12),

$$\sum_{k} (k^{2}/2) \int dx |\chi_{k}(x)|^{2} = \frac{1}{2} \sum_{k} \int dx \left| \frac{d}{dx} \chi_{k}(x) \right|^{2} - \frac{1}{2}K \sum_{k} \int dx \psi^{2}(x) |\chi_{k}(x)|^{2} - \frac{1}{2}K \sum_{k} \int dx \psi^{2}(x) [\eta_{k}(x)\chi_{k}(x) + \eta_{k}^{*}(x)\chi_{k}^{*}(x)],$$

$$\sum_{k} (2\omega_{n} - \frac{1}{2}k^{2}) \int dx |\eta_{k}(x)|^{2} = \frac{1}{2} \sum_{k} \int dx \frac{d}{dx} |\eta_{k}(x)|^{2} - \frac{1}{2}K \sum_{k} \int dx \psi^{2}(x) [\eta_{k}(x)\chi_{k}(x) + \eta_{k}^{*}(x)\chi_{k}^{*}(x)],$$

$$(4.13)$$

$$-2K \sum_{k} \int dx \psi^{2}(x) |\eta_{k}(x)|^{2} - \frac{1}{2}K \sum_{k} \int dx \psi^{2}(x) [\eta_{k}(x)\chi_{k}(x) + \eta_{k}^{*}(x)\chi_{k}^{*}(x)],$$

to reduce the energy to the simpler expression [cf. (3.9)]

$$E_n = E_c(n, m_n) + \frac{1}{2} \frac{d}{dn} \left[\frac{1}{2} K \int dx \, \psi^4(x) \right] + \sum_k \left(\omega_n - \frac{1}{2} k^2 \right) \int |\eta_k(x)|^2.$$
(4.14)

We then turn to the solution of (4.12). In terms of the dimensionless variables

$$z = \frac{1}{2}Knx$$
, $\nu = (2/Kn)k$, (4.15)

and introducing the values of $\psi_n(x)$ and ω_n explicitly, we have in place of (4.13) the dimensionless forms

$$\nu^{2}\chi_{\nu} = -\frac{d^{2}}{dz^{2}}\chi_{\nu} - \frac{4}{\cosh^{2}z}\chi_{\nu} - \frac{2}{\cosh^{2}z}\eta_{\nu}^{*},$$

$$(-2 - \nu^{2})\eta_{\nu}^{*} = -\frac{d^{2}}{dz^{2}}\eta_{\nu}^{*} - \frac{4}{\cosh^{2}z}\eta_{\nu}^{*} - \frac{2}{\cosh^{2}z}\chi_{\nu}.$$
(4.16)

Equation (4.16) has two bound-state solutions which do not correspond to any real physical state but rather express our failure to conserve both momentum and particle number in lowest approximation. These will be discussed in Appendix B.

We consider here the usual scattering solution defined by the condition

$$\lim_{z \to -\infty} \chi_{\nu}^{(+)}(z) = \frac{1}{\sqrt{L}} e^{i\nu z} , \qquad (4.17)$$

where L is the length of the line to which the system is confined. This solution, containing no re-

flected wave, is

$$\chi_{\nu}^{(+)}(z) = \frac{e^{i\nu z}}{L^{1/2}} \frac{1}{(\nu^2 - 1) - 2i\nu} \times \left(\nu^2 - 1 + 2i\nu \tanh z + \frac{1}{\cosh^2 z}\right),$$

$$\eta_{\nu}^{(+)*}(z) = \frac{e^{i\nu z}}{L^{1/2}} \frac{1}{(\nu^2 - 1) - 2i\nu} \frac{1}{\cosh^2 z}.$$
(4.18)

We notice that¹⁰

$$\lim_{z \to \infty} \chi_{\nu}^{(+)}(z) = \frac{e^{i\nu z}}{L^{1/2}} e^{2i\,\delta(\nu)}, \qquad (4.19)$$

where

$$\delta(\nu) = \tan^{-1} [2\nu/(\nu^2 - 1)]. \qquad (4.20)$$

We also notice that

$$\lim_{L \to \infty} \int_{-L/2}^{L/2} \left[|\chi_{\nu}|^2 - |\eta_{\nu}|^2 \right] dx = 1.$$
 (4.21)

At the moment, we require from solution (4.18) only the value of the last term of (4.14). With the usual replacement

$$\sum_{k} - L \int \frac{dk}{2\pi}, \qquad (4.22)$$

we find

$$\sum_{k} (\omega - \frac{1}{2}k^2) \int |\eta_k(x)|^2 = -\frac{1}{12}K^2n^2.$$
 (4.23)

If we combine this with (3.9), we find

$$E_{n} = -\frac{1}{24}K^{2}n^{3}[1 + O(n^{-2})]. \qquad (4.24)$$

This result is as far as we shall go in this paper. The remainder of our discussion will be devoted first to a substantiation of the method utilized thus far and second to several partially independent recalculations of (4.24), the purpose of which is to deepen our understanding of technique.

V. MODIFICATIONS FROM CENTER-OF-MASS MOTION

In effect, we start all over and take into account the motion of the n-particle bound states. Consider the equation of motion for the matrix element

$$\Psi_{n, p}(x) = \frac{1}{2\pi} \int dp' e^{i(p'-p)x} \langle n-1(p) | \psi(0) | n(p') \rangle.$$
(5.1)

Assuming that the energy of the state $|n(p)\rangle$ is exactly of the form

$$E_n(p) = E_n(0) + (p^2/2M_n), \qquad (5.2)$$

$$M_n \equiv mn , \qquad (5.3)$$

for which there is a well-known elementary proof, we derive from the equation of motion (1.5)

$$\left| \omega_n + \left[\left(-i \frac{d}{dx} + p \right)^2 / 2M_n \right] - \left(\frac{p^2}{2M_{n-1}} \right) \right\} \Psi_{np}(x)$$
$$= -\frac{1}{2} \frac{d^2}{dx^2} \Psi_{np}(x) + \text{interaction term}. \quad (5.4)$$

The transformation

$$\Psi_{np}(x) = \exp[ipx/(n-1)]\Psi_n(x), \qquad (5.5)$$

where the implied p independence of the second factor is to be verified (it is in fact a general consequence of Galilean invariance), reduces (5.5) to the form

$$\omega_n \psi_n(x) = -\frac{1}{2m_n} \frac{d^2}{dx^2} \psi_n(x) + \exp[-ipx/(n-1)] \times (\text{interaction term}).$$
(5.6)

The interaction term is, in fact,

$$e^{-i(p_{\mathbf{x}}/n-1)}(-K)\int \frac{dp'}{2\pi}e^{i(p'-p)_{\mathbf{x}}}\sum_{p''p'''} \langle p | \psi^{\dagger}(0) | p'' \rangle \langle p'' | \psi(0) | p''' \rangle \langle p''' | \psi(0) | p' \rangle, \qquad (5.7)$$

where the n dependence has been suppressed. The utilization of the inverse of (5.1) and the ansatz (5.5) proves the latter to be viable, and we obtain as our final result

$$\omega_n \psi_n(x) = -\frac{1}{2m_n} \frac{d^2}{dx^2} \psi_n(x) - K \frac{(n-2)}{(n-1)} \left| \psi_{n-1} \left(\frac{n}{n-1} x \right) \right|^2 \psi_n(x) . \quad (5.8)$$

The function defined by (5.8) differs slightly from

the previously defined classical solution. This distinction will be maintained by writing $\psi_n^{(0)}(x)$ for the latter or even $\psi_n^{(0)}(x,m)$ and $\psi_n^{(0)}(x,m_n)$ to render a further distinction. Here we note that

$$\psi_n^{(0)}(x,m) = \frac{1}{2} \frac{(Km)^{1/2} n}{\cosh(\frac{1}{2}Kmnx)},$$
(5.9)

having returned the mass explicitly to the expression in order to aid the reader to follow the subsequent argument. To appreciate the significance of (5.5), we recalculate the various physical quantities

$$nL = \left\langle n(p) \left| \int dx \, \psi^{\dagger}(x) \psi(x) \left| n(p) \right\rangle \right\rangle$$
$$\cong \sum_{p'} \left\langle n(p) \left| \psi^{\dagger}(0) \right| n - 1(p') \right\rangle$$
$$\times \left\langle n - 1(p') \left| \psi(0) \right| n(p) \right\rangle L, \qquad (5.10)$$

$$E_n(p)L \equiv \langle n(p) | H | n(p) \rangle.$$
(5.11)

Repeating the type of reasoning which led to (5.8), we find

$$\int dx \,\psi_n^2(x) = n^2/(n-1) \,, \qquad (5.12)$$

$$E_n(p) = (p^2/2mn) + E_n(0), \qquad (5.13)$$

$$E_{n}(0) = \left(\frac{n-1}{n}\right)^{3} \frac{1}{2} \int dx \left(\frac{d}{dx}\psi_{n}\right)^{2}$$
$$-\frac{1}{2}K\left(\frac{n-2}{n}\right) \int dx \psi_{n}^{2}(x)\psi_{n-1}^{2}\left(\frac{n}{n-1}x\right).$$
(5.14)

Equations (5.8) and (5.12)–(5.14) describe correctly the results of recoil and *n* fluctuation. They can therefore be used to justify the corresponding calculation of Sec. IV. This can be done in several equivalent ways. A little thought (or possibly a lot of thought) will convince the reader that it suffices to insert into (5.14) Eq. (5.9) multiplied by $[n/(n-1)]^{1/2}$, the factor needed to renormalize to (5.12), and then to expand the corresponding energy expression in powers of n^{-1} . This same procedure may be reformulated as follows: First, with ψ_n as just defined, an elementary exercise tells us that (5.12) is equivalent to the expression

$$\int dx \,\psi_n^{(0)}(x, m_n)^2 = n \,. \tag{5.15}$$

This suggests that we rewrite (5.14) in terms of the function $\psi_n^{(o)}(x, m_n)$. We thus find by another elementary exercise

$$E_n(0) = \left(\frac{n-1}{n}\right)^3 E_c(n, m_n).$$
 (5.16)

(The classical calculation may be written

$$E_c = T_c + V_c , \qquad (5.17)$$

$$T_c = -\frac{1}{2}V_c = \frac{1}{24}K^2 m n^3, \qquad (5.18)$$

returning the mass to its place.) It follows that to the first two orders in n, (5.16) may be rewritten

 \mathbf{as}

$$E_{n}(0) = E_{c}(n, m_{n}) - \frac{3}{n}E_{c}(n, m)$$
$$= E_{c}(n, m_{n}) - \frac{3}{2n}V_{c}$$
$$= E_{n}(n, m_{n}) - \frac{1}{2}\frac{d}{dn}V_{c}, \qquad (5.19)$$

in agreement with (3.9).

We conclude this section with one more elementary exercise by calculating the "classical" part of the energy associated with the first two terms of (1.6): Call this E'_n . We find

$$E'_{n} = \left(\frac{n-1}{n}\right)^{3} \frac{1}{2} \int dx \left[\frac{d}{dx}\psi_{n}(x)\right]^{2} - \frac{1}{2}K\left(\frac{n-1}{n}\right)^{2} \int dx \psi_{n}^{4}(x).$$
(5.20)

Further manipulation shows that

$$E'_{n} = E_{n}(0) + (2/n)V_{c}$$

= $-\frac{1}{24}K^{2}n^{3} - \frac{1}{12}K^{2}n^{2}$, (5.21)

which we require for later reference. The last term in $(1.6) \sim \delta(0)$ must be treated with the quantum fluctuations which, term by term, will be infinite in this treatment.

The effect of recoil on the scattering equation (4.12) has also been studied, but the result is needed only in Appendix A, where it will be quoted.

VI. COMPLETENESS AND COMMUTATION RELATIONS

The main result of this section, the completeness relation for the scattering functions of Sec. IV, is needed to carry through the manipulation of the next section. The impatient reader need only be willing to accept the final result, Eq. (6.5).

We derive the relation twice, first by straightforward calculation, second from the commutation relation (1.2). A detailed discussion of the physical significance of certain peculiar terms which occur in it is relegated to Appendix B.

We note that Eqs. (4.12) imply the orthogonality relation

$$\int dx [\chi_{\nu}^{*}(x)\chi_{\nu'}^{*}(x) - \eta_{\nu}(x)\eta_{\nu'}^{*}(x)] = 0, \quad \nu \neq \nu' \quad (6.1)$$

(and we have already discovered that the norm is unity). This suggests that we study the integral

$$C(x, y) = L \int \frac{dk}{2\pi} [\chi_k(x)\chi_k^*(y) - \eta_k(x)\eta_k^*(y)]. \quad (6.2)$$

The integral over k is readily evaluated, and we find

$$C(x, x') = \delta(x - x') + \frac{1}{2}Kne^{-|z-z'|} \left[(|z - z'| - 1)(1 - \tanh z \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z') + \epsilon(z - z')(|z - z'| - 1)(\tanh z - \tanh z')$$

$$-\frac{1}{2}|z-z'|\left(\frac{1}{\cosh^2 z}+\frac{1}{\cosh^2 z'}\right)-\frac{1}{2}(z-z')\left(\frac{\tanh z}{\cosh^2 z'}-\frac{\tanh z'}{\cosh^2 z}\right)\right],$$
(6.3)

where $\epsilon(x)$ is the sign function. With the help of the identity

 $\exp(-|x-y|) = \cosh x \cosh y - \sinh x \sinh y - \epsilon(x-y) \sinh x \cosh y + \epsilon(x-y) \cosh x \sinh y, \qquad (6.4)$

(6.3) can be reduced to the form (through straightforward but slightly tedious algebra)

$$C(x, x') = \delta(x - x') - \frac{\partial}{\partial n} \psi_n(x) \psi_n(y) + \frac{1}{n} \left(x \frac{\partial}{\partial y} + y \frac{\partial}{\partial x} \right) \psi_n(x) \psi_n(y) , \qquad (6.5)$$

with ψ_n given by (5.9), for example. Equivalent forms used later may be obtained from the identity

$$\frac{\partial}{\partial n}\psi_n(x) = \frac{1}{n}\psi_n(x) + \frac{x}{n}\frac{\partial}{\partial x}\psi_n(x).$$
(6.6)

We next verify (6.5) with the help of the commutator

$$\lim_{p \to 0} \langle n(p) | [\psi(x), \psi^{\dagger}(y)] | n(p) \rangle = \lim_{p \to 0} \langle p | p \rangle \delta(x - y)$$
$$= L\delta(x - y).$$
(6.7)

A consistent approximation to (6.7) is to include number conservation and momentum conservation for the bound intermediate states but to ignore it for the scattering states, the same approximation that has been made throughout. We thus find

$$\int d\xi \sum_{k} \left[\chi_{k}(x+\xi)\chi_{k}^{*}(y+\xi) - \eta_{k}(x+\xi)\eta_{k}^{*}(y+\xi) \right] + \psi_{n+1}(x+\xi)\psi_{n+1}(y+\xi) - \left(\frac{n-1}{n}\right)\psi_{n}(x+\xi)\psi_{n}\left(y+\xi+\frac{1}{n}(x-y)\right) \\ = \int d\xi \,\delta(x-y) \,. \quad (6.8)$$

The terms depending on ψ_n are to leading order

$$\int d\xi \left\{ \frac{\partial}{\partial n} \left[\psi_n(x+\xi)\psi_n(y+\xi) \right] - \frac{1}{n} \psi_n(x+\xi)\psi_n(y+\xi) - \frac{1}{n} (x-y) \frac{\partial}{\partial y} \left[\psi_n(x+\xi)\psi_n(y+\xi) \right] \right\}$$
$$= \int d\xi \left\{ \frac{\partial}{\partial n} \left[\psi_n(x+\xi)\psi_n(y+\xi) \right] - \frac{1}{n} \left[(x+\xi) \frac{\partial}{\partial x} + (y+\xi) \frac{\partial}{\partial y} \right] \psi_n(x+\xi)\psi_n(y+\xi) \right\}, \quad (6.9)$$

the eqivalence of the two forms following upon integration by parts. The resulting integrand of (6.8) can now be required to be independent of ξ , whence (6.5) is regained.

Since only (6.5) is needed for the calculations which follow, further discussion is relegated to Appendix B.

VII. ALTERNATE CALCULATION OF FIRST QUANTUM CORRECTION

With the help of the completeness condition (6.5), we now give a new account of the first quantum

correction, utilizing as a basis the form (1.6) of the Hamiltonian. This calculation has elements quite analogous to those which occur in relativistic field theories requiring renormalization. We shall thereby establish the soundness of our approach for application to such cases.

Starting from Eq. (1.6) and utilizing the standard reasoning, we obtain a new expression for $E_n(0)$, namely

(7.1)

$$E_{n}(0) = E_{n}' + \frac{1}{2}K\delta(0)n - \omega \sum_{k} \int dx |\eta_{k}(x)|^{2} + \frac{1}{2} \sum_{k} \int dx \left| \frac{d}{dx} \eta_{k}(x) \right|^{2} - K \sum_{k} \int dx \psi^{2}(x) \left[\frac{3}{2} |\eta_{k}(x)|^{2} + \frac{1}{2} |\chi_{k}(x)|^{2} + \frac{1}{2} \chi_{k}(x) \eta_{k}(x) + \frac{1}{2} \chi_{k}^{*}(x) \eta_{k}^{*}(x) \right],$$

where E'_n is given by (5.21).

This can be rewritten for our needs with the help of a special case of (6.5), namely

$$\sum_{k} \left[\left| \chi_{k}(x) \right|^{2} - \left| \eta_{k}(x) \right|^{2} \right] = \delta(0) - \frac{2}{n} \psi_{n}^{2}(x) ,$$

and with the help of (4.12), where the aim is to eliminate the interaction terms in (7.1). We thus find

$$E_{n}(0) = E'_{n} + (2/n) V_{c} + K\delta(0)n$$

$$+ \frac{1}{2} \sum_{k} \int dx \frac{1}{2}k^{2} [|\chi_{k}(x)|^{2} - |\eta_{k}(x)|^{2}]$$

$$- \frac{1}{2} \sum_{k} \int dx \frac{1}{2} [|\partial_{x}\chi_{k}(x)|^{2} - |\partial_{x}\eta_{k}(x)|^{2}].$$
(7.3)

Though (7.3) is not the final form sought, we check it, nevertheless, by explicit introduction of the solutions (4.18). Each of the last two terms of (7.3) is cubically divergent, but these leading divergences cancel, leaving, after a small calculation, the expression

$$-\frac{1}{2}K^2n^2\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\frac{\nu^2}{(\nu^2+1)}.$$
(7.4)

When combined with the term

$$K\delta(0)n = \frac{1}{2}K^2n^2 \int_{-\infty}^{\infty} \frac{d\nu}{2\pi},$$
 (7.5)

we obtain a finite sum and value $\frac{1}{4}K^2n^2$ which leads again to a complete cancellation of $O(n^2)$ terms in (7.3).

We now have our final go at (7.3). In the penultimate term, we introduce the normalization (4.21). For the last term, we use yet another special case of the completeness relation,

$$\sum_{k} \left[\left| \partial_{x} \chi_{k}(x) \right|^{2} - \left| \partial_{x} \eta_{k}(x) \right|^{2} \right]$$
$$= \lim_{x \to y} \partial_{x} \partial_{y} \delta(x - y) - \frac{4}{n} \left[\partial_{x} \psi(x) \right]^{2} + \frac{2}{n} \psi(x) \frac{\partial^{2}}{\partial x^{2}} \psi(x) .$$
(7.6)

When Eq. (7.6) is introduced into (7.3), the last two terms of the former yield a contribution $\frac{1}{8}K^2n^2$. By consequence of all of the above, (7.3) is transformed into the expression

 $E_n(0) = -\frac{1}{24}K^2n^3 - \frac{1}{8}K^2n^2 + \delta E_n, \qquad (7.7)$

with

$$\delta E_n = \frac{1}{2} \sum_k \frac{1}{2}k^2 - \frac{1}{2} \sum_{k'} \frac{1}{2}(k')^2 + K\delta(0)n , \qquad (7.8)$$

where the first sum is over the k values of the interacting system in a box and the second is the

corresponding sum for the noninteracting system. Following a standard argument, we have

$$k_p'L = 2p\pi,\tag{7.9}$$

$$k_p L + 2\delta = 2p\pi$$

or

$$k_{p} \cong k'_{p} - (2\delta/L)$$
. (7.10)

Remembering also (7.3), this yields altogether

$$\delta E_n = -\frac{1}{4}K^2 n^2 \int_{-\infty}^{\infty} \frac{\nu d\nu}{2\pi} \left[\delta(\nu) - (2/\nu) \right], \qquad (7.11)$$

where $\delta(\nu)$ is given by (4.20). The integral (7.11) is again finite and conveniently reduced by integration by parts to the form

$$\delta E_n = \frac{1}{4} K^2 n^2 \int \frac{d\nu}{2\pi} \frac{1}{\nu^2 + 1}$$
$$= \frac{1}{8} K^2 n^2 , \qquad (7.12)$$

the required result.

VIII. CUBIC SCHRÖDINGER EQUATION FOR FERMIONS

Let us now interpret the field $\psi(x)$ as an *N*-component fermion field $\psi_i(x)$, $i=1,\ldots,N$. Thus we replace (1.1) and (1.2) by the expressions (summation convention)

$$H = \frac{1}{2} \int dx \frac{d}{dx} \psi_i^{\dagger}(x) \frac{d}{dx} \psi_i(x)$$
$$- \frac{1}{2}K \int dx \psi_i^{\dagger}(x) \psi_j^{\dagger}(x) \psi_j(x) \psi_i(x) , \qquad (8.1)$$

$$\left\{\psi_{i}(x), \psi_{j}^{\dagger}(y)\right\} = \delta_{ij}\delta(x-y) , \qquad (8.2)$$

and (1.4) becomes

$$\int dx \,\psi_i^{\dagger}(x)\psi_i(x) \equiv Q \,. \tag{8.3}$$

If we consider the ground state for any n < N, it is degenerate; the different states are labeled $|i_1 \cdots i_n\rangle$, where $i_1 \cdots i_n$ is an ordered set of distinct integers from the set $1 \cdots N$. The matrix element with which we would begin our study,

$$\langle i'_1 \cdot \cdot \cdot i'_{n-1} | \psi_j(x) | i_1 \cdot \cdot \cdot i_n \rangle$$
, (8.4)

is zero unless j is in the set $i_1 \cdots i_n$ and not in the primed set (which otherwise must coincide with the unprimed set). If the indices match properly, the matrix element depends only on the total number and not on the individual indices. A completely analogous simplification occurs for the scattering matrix elements. When these points are taken into account along with the observation that the algebra of the operators played no essential role in the first, finite calculation of the

energy which was carried out in Secs. III-V, we reach the almost immediate conclusion that the Fermi system enjoys the same ground-state energy spectrum as the Bose system. Amusing differences in the completeness relations implied by the algebra will not be discussed here.

APPENDIX A: GALILEAN INVARIANCE AND ENERGY SELF-CONSISTENCY

In the body of this paper we have depended heavily on the existence of number conservation. Indeed it served an essential role as quantization condition, as exemplified by Eq. (4.10). However, this raises the problem of how one can proceed in theories without number conservation or equivalent (such as neutral scalar theories). It is comforting, therefore, to be able to prove that the same normalization condition emerges from the insistence on Galilean invariance.

We first recall the elementary basis for such considerations translated into the language of second quantization: In terms of the center-ofmass operator

$$\hat{N}\hat{X} = \int dx \,\psi^{\dagger}(x)x\psi(x) , \qquad (A1)$$

the state

$$|n(p)\rangle = e^{-iXp}|n(0)\rangle \tag{A2}$$

has the energy $E_n(0) + (p^2/2nm)$. We must then demand that when we calculate $\langle n(p) | H | n(p) \rangle$ by the sum over states method we reproduce the p^2 term exactly.

In our calculation the coefficient of $(p^2/2m)$ will present itself as a power series in n^{-1} . We require that the leading term be n^{-1} and that all higher-order terms vanish. To reproduce (4.10) we shall need terms of order n^{-2} in this series.

For this purpose we must include center-ofmass motion in the scattering functions. We only quote the needed results: Defining the amplitudes

$$X(x,k,p) = \int \frac{dp'}{2\pi} e^{i(p'+k-p)x} \times \langle (n-1)(p) | \psi(0) | (n-1)(p'), k \rangle,$$
(A3)

$$Y^{*}(x,k,p) = \int \frac{dp'}{2\pi} e^{i(p'+k-p)x} \\ \times \langle n(p) | \psi^{\dagger}(0) | (n-2)(p'), k \rangle, \quad (A4)$$

by studying the equations of motion for these coupled quantities, we can show that to *leading order* in the corrections

$$X(x, k, p) \cong e^{i(p-k)x/n} \chi_{k-(p/n)}(x)$$
, (A5)

$$Y^{*}(x, k, p) \cong e^{i(p-k)x/n} \eta^{*}_{k-(p/n)}(x) , \qquad (A6)$$

where, in particular, it is the result (A6) that is needed below.

At this point we then repeat and extend the calculation summarized in (5.2)-(5.14) including all the quantum fluctuation contributions to first order order. The quantity $E_n(0)$ is unaffected. The term proportional to p^2 yields the condition

$$\frac{p^2}{2nm} = \frac{p^2}{2m} \left[\frac{n-1}{n^3} \int dx \, \psi_n^2(x) + \frac{1}{n^2} \sum_k \int dx \, |\eta_k(x)|^2 \right].$$
(A7)

To the required order this implies (4.10).

APPENDIX B: QUANTUM THEORY OF STABILITY OF PERIODIC ORBITS

The scattering equations (4.12) are rewritten as

$$\epsilon \chi = -\frac{1}{2m} \frac{d^2}{dx^2} \chi - K(2\psi^2 \chi + \psi^2 \eta^*) - \omega \chi ,$$
(B1)

$$-\epsilon \eta^* = -\frac{1}{2m} \frac{d^2}{dx^2} \eta^* - K(2\psi^2 \eta^* + \psi^2 \chi) - \omega \eta^* ,$$

where

$$\epsilon = \frac{1}{2m} k^2 - \omega \,. \tag{B2}$$

Equations (B1) have the matrix form (τ_i are Pauli matrices)

$$\epsilon \tau_3 Z = MZ$$
, (B3)

$$Z = \begin{pmatrix} \chi \\ \eta^* \end{pmatrix}, \tag{B4}$$

and M is a Hermitian differential operator matrix. In general, an equation of the form (B3) may have both bound and continuum solutions. In order not to have to make the distinction in the formal discussion that follows, we imagine "box" normalization. The solutions of (B3) possess a number of interesting properties. Most proofs are left as exercises.¹¹

(i) Orthogonality. Consider two solutions $Z_{\nu}(\epsilon_{\nu}), Z_{\nu'}(\epsilon_{\nu'})$:

$$\int Z^{\dagger}_{\nu} \tau_3 Z_{\nu'} = 0, \quad \epsilon_{\nu} \neq \epsilon_{\nu'} .$$
 (B5)

(ii) Doubling. To every solution Z_{ν} , ϵ_{ν} there is another solution $\tau_1 Z_{\nu}^*$ with opposed eigenvalue $-\epsilon_{\nu}$. This doubling fails only when $\epsilon_{\nu} = 0$, which occurs in many cases of interest (see below).

(iii) Stability. We return to our particular case. Let us ask for the condition that the semiclassical energy

4

$$E_n = \frac{1}{2m} \int dx \left| \frac{d}{dx} \psi(x) \right|^2$$
$$-\frac{1}{2}K \int \left[|\psi(x)|^2 \right]^2$$
(B6)

be a local minimum for states of a given n. We investigate this condition by introducing into (B6) the comparison functions

$$\begin{aligned} \psi &\rightarrow \psi + \beta ,\\ \psi^* &\rightarrow \psi^* + \beta^* , \end{aligned} \tag{B7}$$

subject to the condition

$$\int (\psi^* + \beta^*)(\psi + \beta) = \int \psi^* \psi = n .$$
 (B8)

A straightforward calculation, utilizing (B8) and the equation satisfied by ψ , shows that for small β

$$E_n(\psi+\beta) - E_n(\psi) = \frac{1}{2} \int dx \ B^{\dagger}(x) \ MB(x) , \qquad (B9)$$

$$B(x) = \begin{pmatrix} \beta(x) \\ \beta^*(x) \end{pmatrix}, \tag{B10}$$

where M is the same matrix as occurs in (B3). The condition for a local minimum is thus that M be positive-definite, i.e., that all its eigenvalues be positive. This is not so in our case, but we shall turn below to the difficulties thus engendered. We first pursue the reasoning associated with the simpler case that M is positivedefinite.

(iv) Sign of norm. From (B3), we then derive

$$\epsilon_{\nu} \int Z_{\nu}^{\dagger} \tau_{3} Z_{\nu} = \int Z_{\nu}^{\dagger} M Z_{\nu} > 0.$$
 (B11)

Thus the sign of the norm $\int Z_{\nu}^{\dagger} \tau_{3} Z_{\nu}$ is the sign of the energy. We designate the pairs as Z_{ν^+} , $Z_{\nu} - = \tau_1 Z_{\nu^+}^*$.

(v) Completeness. If M is Hermitian and positive-definite, the solutions of (B3) satisfy the completeness condition

$$\sum_{\nu} \left[Z_{\nu^+}(x) Z_{\nu^+}^{\dagger}(y) \tau_3 - Z_{\nu^-}(x) Z_{\nu^-}^{\dagger}(y) \tau_3 \right] = \mathbf{1} \delta(x - y) .$$
(B12)

(vi) Normalization. From (B5) and (B12) we learn

$$\int Z_{\nu^{\pm}}^{\dagger} \tau_{3} Z_{\nu^{\pm}} = \pm 1 .$$
 (B13)

(vii) Zero eigenvalues. We first consider the situation for our special case (B1). We can find

two independent solutions for $\epsilon = 0$, namely,

$$Z^{(1)}(x) = \begin{pmatrix} \psi_n(x) \\ -\psi_n(x) \end{pmatrix},$$
 (B14)

$$Z^{(2)}(x) = \begin{pmatrix} d\psi_n/dx \\ d\psi_n/dx \end{pmatrix}.$$
 (B15)

It will later be clear that by consequence of the calculations of Sec. VI there are no others. In contrast to the scattering solutions discussed in Sec. IV, these are not associated with any physical states of the system. They represent "spurious" solutions which signal the fact that the semiclassical solution violates number conservation and momentum conservation, respectively. This is clear from the considerations of Sec. VI in which concordance between the completeness relation computed directly and that inferred from the commutation relation requires precisely this interpretation.

(viii) Altered completeness relation. We turn finally to the problem of how the completeness relation (B12) is altered in the presence of zero eigenvalues. Let there be a set of linearly independent zero-energy solutions $Z^{(i)}$, $i = 1, \ldots, q$ satisfying

$$MZ^{(i)} = 0$$
. (B16)

Assume M is real and that the $Z^{(i)}$ are real. As in (B14) and (B15), the upper and lower components of $Z^{(i)}$ are equal up to a sign, and therefore

$$\int Z^{(i)} \tau_3 Z^{(i)} = 0.$$
 (B17)

We may also assume by construction that

$$\int Z^{(i)} \tau_3 Z^{(j)} = 0, \quad i \neq j$$
(B18)

and of course

$$\int Z_{\nu}^{\dagger} \tau_3 Z^{(i)} = 0, \quad \epsilon_{\nu} \neq 0.$$
(B19)

Let us now imagine that we alter the operator Μ,

$$M \rightarrow M' = M + \delta M (\delta \alpha_1 \cdots \delta \alpha_q), \qquad (B20)$$

where M' is positive-definite, but q of the eigenvalues are small. Let the vectors (2q of them) associated with the small eigenvalues be designated $Z_{+}^{(i)}$. The passage to zero eigenvalues requires a rescaling of the solutions because of the discontinuous jump in norm from ± 1 to 0. This rescaling is most easily investigated in terms of different functions, as we see below.

In the limit of zero eigenvalue, we lose one

solution. By suitable choice of phases, let us take the surviving solution as the limit of the sum

$$Z_{e}^{(i)} = \frac{1}{2^{1/2}} \left(Z_{+}^{(i)} + Z_{-}^{i} \right) , \qquad (B21)$$

and suppose that

$$Z_{o}^{(i)} = \frac{1}{2^{1/2}} \left(Z_{+}^{(i)} - Z_{-}^{(i)} \right) \to 0 .$$
 (B22)

The three orthonormalization conditions involving $Z_{+}^{(i)}$ translate into

$$\int Z_e^{(i)} \tau_3 Z_e^{(i)} = \int Z_o^{(i)} \tau_3 Z_o^{(i)} = 0 , \qquad (B23)$$

$$\int Z_e^{(i)} \tau_3 Z_o^{(i)} = \int Z_o^{(i)} \tau_3 Z_e^{(i)} = 1.$$
 (B24)

If we examine the contribution of these terms to the completeness relation, we find

$$Z_{+}^{(i)}(x)Z_{+}^{i\dagger}(y)\tau_{3} - Z_{-}^{(i)}(x)Z_{-}^{(i)\dagger}(y)\tau_{3}$$
$$= Z_{e}^{(i)}(x)Z_{o}^{(i)\dagger}(y)\tau_{3} + Z_{o}^{(i)}(x)Z_{e}^{(i)\dagger}(y)\tau_{3}.$$
(B25)

In the limit $\epsilon^{(i)} \rightarrow 0$, $Z_o^{(i)} \rightarrow 0$, but the discontinuity of the conventional norm forces $Z_e^{(i)} \rightarrow \infty$. However, the structure of (B24) and (B25) suggests that it may be possible to rescale these quantities so that their product is and remains finite.

This can be substantiated precisely by studying the limit of the equations

$$\pm \epsilon^{(i)} \tau_3 Z_{\pm}^{i} = (M + \delta M) Z_{\pm}^{(i)} . \tag{B26}$$

Utilizing (B21) and (B22), we replace (B26) by the appropriate sum and difference equations, which up to higher-order terms become

$$MZ_e^{(i)} \cong 0 , \tag{B27}$$

$$MZ_{a}^{(i)} = \epsilon^{(i)} \tau_{3} Z_{e}^{(i)} . \tag{B28}$$

Now if (B24) and (B25) are to have a finite limit and (B27) and (B28) are to be finite after rescaling, the only possible solution is that the quantities

$$Z^{(i)} \equiv (\epsilon^{i})^{1/2} Z_{e}^{(i)} , \qquad (B29)$$

$$Y^{(i)} = Z_{o}^{(i)} / (\epsilon^{i})^{1/2}$$
(B30)

have finite limits. This yields the equations

$$\int Z^{(i)} \tau_3 Z^{(i)} = \int Y^{(i)} \tau_3 Y^{(i)} = 0,$$

$$\int Z^{\dagger}_{\nu} \tau_3 Z^{(i)} = \int Z^{\dagger}_{\nu} \tau_3 Y^{(i)} = 0,$$
(B31)

$$\int Y^{(i)} \tau_3 Z^{(i)} = 1 , \qquad (B32)$$

$$MZ^{(i)} = 0$$
, (B33)

and

$$MY^{(i)} = \tau_3 Z^{(i)} . \tag{B34}$$

These equations determine an auxiliary set of functions $Y^{(i)}$, needed to form a complete set of functions.

To summarize: When there are zero eigenvalues the completeness relation reads

$$\sum_{\nu} \left[Z_{\nu^{+}}(x) Z_{\nu^{+}}^{\dagger}(y) \tau_{3} - Z_{\nu^{-}}(x) Z_{\nu}^{\dagger} - (y) \tau_{3} \right] + \sum_{i} \left[Z^{(i)}(x) Y^{(i)\dagger}(y) \tau_{3} + Y^{(i)}(x) Z^{(i)\dagger}(y) \tau_{3} \right] = \delta(x - y) \mathbf{1} , \qquad (B35)$$

where the $Y^{(i)}$ satisfy (up to a possible scale)

$$MY^{(i)} = \tau_3 Z^{(i)} , \qquad (B36)$$

$$\int Y^{(i)} \tau_3 Y^{(i)} = 0,$$
(B37)
$$\int Y^{(i)} \tau_0 Z^{(i)} = 1.$$

To illustrate this formulation, we return to our

special example, where it is easy to show that

$$Y^{(1)}(x) = \tau_3 \frac{\partial Z^{(1)}(x)}{\partial n}$$
, (B38)

$$Y^{(2)}(x) = -\frac{x}{n} Z^{(1)}(x)$$
(B39)

satisfy (B36). Aside from the direct solution of (B36), we verify (B38) and (B39) by showing that when inserted into (B35) they yield the completeness condition (4.5). This is so.

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