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Second Quantization in a Waveguide with Variable Cross Section

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The motion of a system consisting of noninteracting bosons in a waveguide with variable cross section is studied. These particles have transverse as well as longitudinal degrees of freedom, but only a finite number of transverse modes can propagate in the waveguide. While for a waveguide with constant cross section, the numbers of particles in a given state of longitudinal and transverse modes remain constant, in the case of a waveguide with variable cross section there is conversion between these modes, although the total number of particles is conserved. By considering the equations of motion for the annihilation (or creation) operator, it is shown that the boundaries act as an external force, and thus generate localized transverse modes in the waveguide.

1. INTRODUCTION

When a stream of bosons or fermions flows along a pipe or a tube (here called a waveguide) then the boundaries impose additional forces (forces of constraint) (van Kampen, 1984) on the motion of these particles. For static boundaries and for a specific geometry where the Schrödinger equation is separable and solvable, one observes that these forces are responsible for a shift in the phase of the incident wave when there is a constriction along the direction of the flow of the particles (Levy-Leblond, 1987; Razavy, 1989) and that the effective force is nonlocal (Razavy, 1989). On the other hand, if the cross section of the waveguide changes with time, the energies of the particles are directly affected by the motion of the walls (Razavy, 1993, 1994). The geometrical change in the boundaries also creates localized or propagating modes that are not present in the incoming beam of the particles. The study of this aspect of the change of the boundary in the case of a long

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waveguide is the subject of the present work. Here the formalism of the second quantization is applied to study the motion of these particles. There are a number of very interesting physical systems where the present formulation can be applied. For instance, the theory of quantum conduction through a constriction (Szafer and Stone, 1989) and two-dimensional quantum wires (Wu *et al.*, 1992, and references therein) are just two examples of such systems.

In Section 2, we start with the Hamiltonian operator, and write it in terms of creation and annihilation operators. These operators depend on two transverse and one longitudinal quantum numbers. The first two are discrete and bounded and are connected to the finite cross section of the waveguide and the energy of the incoming particles, and the third, the longitudinal mode, is associated with the translational motion of the particles along the waveguide. We also assume that the waveguide extends from $z = -\infty$ to $z = +\infty$ and is symmetric about $z = 0$. This last requirement is not essential for the present formulation, but it simplifies the calculation. In Section 3, we find the equation of motion for the creation and annihilation operators and show that while the total number of particles is conserved, the number of particles with a given transverse or longitudinal quantum number does not remain constant in the course of motion. We also obtain the integral equation for the single-particle wavefunction in momentum space, which shows the coupling between the transverse and longitudinal modes. By solving this integral equation approximately we show that if there is a gradual increase in the cross section followed by a gradual decrease, then there will be localized modes appearing around the point where the cross section is maximum; this is similar to the result obtained for acoustic waveguides.

2. THE HAMILTONIAN OPERATOR

Let us consider a waveguide bounded by the planes $x = -1$, $x = 1$, $y = 0$, and $y = L(z)$, with particles satisfying Bose statistics entering the waveguide from $z = -\infty$ and leaving at $z = \infty$. We assume that $L(z)$ is an even function of z, and that asymptotically it tends to a well-defined nonzero value L_a, i.e.,

$$\lim L(z) \to L_a \qquad \text{as} \quad |z| \to \infty \tag{2.1}$$

The Hamiltonian for this system is given by ($\hbar = 1$)

$$H = (1/2M) \int_{-\infty}^{\infty} dz \int_{0}^{L(z)} dy \int_{-1}^{1} dx \, (\nabla\psi^*) \cdot (\nabla\psi) \tag{2.2}$$

where M is the mass of each particle. The operators ψ^* and ψ must vanish at the boundaries; therefore we can expand both in terms of Fourier series,

$$\psi(x, y, z, t) = [1/\pi L(z)]^{1/2} \int_{-\infty}^{\infty} e^{ipz} dp \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_{nm}(p, t) \times \{\sin[n\pi y/L(z)] \cos[(m + 1/2)\pi x]\} \tag{2.3}$$

$$\psi^*(x, y, z, t) = [1/\pi L(z)]^{1/2} \int_{-\infty}^{\infty} e^{iqz} dq \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} a_{jl}^*(q, t) \times \{\sin[j\pi y/L(z)] \cos[(l + 1/2)\pi x]\} \tag{2.4}$$

In these equations $a_{jl}^*(q, t)$ and $a_{nm}(k, t)$ are creation and annihilation operators. They satisfy the equal-time commutation relations

$$[a_{nm}(p, t), a_{jl}^*(q, t)] = \delta_{nj}\delta_{ml}\delta(p - q) \tag{2.5}$$

and

$$[a_{nm}^*(p, t), a_{jl}^*(q, t)] = [a_{nm}(p, t), a_{jl}(q, t)] = 0 \tag{2.6}$$

By substituting (2.3) and (2.4) in (2.2) and carrying out the integration, we find

$$\begin{aligned} H = \sum_{m=0}^{\infty} (1/2M) \Bigg\{ \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dp \, [p^2 + (n^2\pi^2/L_a^2) \\ + (m + 1/2)^2] a_{nm}^*(p, t) a_{nm}(p, t) \\ + \sum_{n=0}^{\infty} \sum_{j=0}^{\infty} \pi n j B_{nj} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dq \, dk \, F(p - q) a_{jm}^*(q, t) a_{nm}(p, t) \\ + \sum_{n=0}^{\infty} (n^2\pi^2/L_a^2) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dq \, dp \, K(p - q) a_{nm}^*(q, t) a_{nm}(p, t) \\ + \sum_{n=0}^{\infty} \sum_{j=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dq \, dp (qn + pj) A_{jn} G(p - q) a_{jm}^*(q, t) a_{nm}(p, t) \Bigg\} \end{aligned} \tag{2.7}$$

The quantities appearing in this expression for H are defined by

$$F(p) = \int_{-\infty}^{\infty} \exp(ipz)[(dL/dz)/L]^2 \, dz \tag{2.8}$$

$$G(p) = \int_{-\infty}^{\infty} p \exp(ipz) \log[L(z)/L_a] \, dz \tag{2.9}$$

$$K(p) = \int_{-\infty}^{\infty} \exp(ipz)\{1/[L(z)]^2 - 1/[L_a]^2\} \, dz \tag{2.10}$$

$$B_{nj} = 2(-1)^{j+n}(j^2 + n^2)/[\pi^2(j^2 - n^2)^2], \qquad n \neq j \tag{2.11}$$

$$B_{nn} = (1/6) + 1/(4n^2\pi^2) \tag{2.12}$$

$$A_{jn} = (-1)^{j+n}j/[\pi(n^2 - j^2)], \qquad n \neq j \tag{2.13}$$

and

$$A_{nn} = -1/(4n\pi) \tag{2.14}$$

Since states with different quantum numbers m do not couple, we can write H as the sum

$$H = \sum_{m=0}^{\infty} H_m \tag{2.15}$$

where H_m is the operator defined by the quantity in the curly brackets in (2.7). From this point on we suppress the index m and consider H_m for a fixed m value.

3. EQUATIONS OF MOTION

In addition to the Hamiltonian H, there is a conserved quantity which is given by the expectation value of the number operator N,

$$N = \sum_{j=0}^{\infty} \int_{-\infty}^{\infty} a_j^*(p, t)a_j(p, t)\, dp \tag{3.1}$$

Using the commutation relation

$$[a_j^*(p, t)a_j(p, t), a_k^*(q, t)a_n(r, t)] = a_j^*(p, t)a_n(r, t)\delta_{jk}\delta(p - q) - a_k^*(q, t)a_j(p, t)\delta_{jn}\delta(r - p) \tag{3.2}$$

we find that

$$i(dN/dt) = [N, H] = 0 \tag{3.3}$$

But the number in each discrete j mode, i.e.,

$$N_j = \int_{-\infty}^{\infty} a_j^*(p, t)a_j(p, t)\, dp \tag{3.4}$$

does not remain constant, i.e., we have conversion from the continuous mode p to the discrete mode j and vice versa. The equation of motion for $a_j(p, t)$ is given by the Heisenberg equation

$$i[da_j(p, t)/dt] = (1/2M)[p^2 + (j^2\pi^2/L_a^2)]a_j(p, t) + (1/2M) \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \Gamma_{jn}(p, q)a_n(q, t)\, dq = 0 \tag{3.5}$$

where

$$\Gamma_{jn}(p, q) = (j^2\pi^2/L_a^2)\delta_{jn}K(p - q) + \pi jnB_{jn}F(p - q) - \pi(pn + qj)A_{jn}G(p - q) \tag{3.6}$$

The operator equation (3.5) is a linear differential equation for $a_j(p, t)$. By expanding $a_j(p, t)$ in terms of the Fourier integral

$$a_j(p, t) = \int e^{-iEt}a_j(p, E)dE \tag{3.7}$$

we find that $a_j(p, E)$ satisfies the equation

$$[E - \epsilon(j, p)]a_j(p, E) = -(1/2M) \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \Gamma_{jn}(p, q)a_n(q, E)\, dq \tag{3.8}$$

where

$$\epsilon(j, p) = (1/2M)[p^2 + (j^2\pi^2/L_a^2)] \tag{3.9}$$

The expectation value of $a_j(p, E)$

$$\langle 0 | a_j(p, E) | 1_{jp}\rangle = u_j(p, E) \tag{3.10}$$

also satisfies an equation similar to (3.8) and is the solution of the integral equation

$$[E - \epsilon(j, p)]u_j(p, E) = -(1/2M) \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \Gamma_{jn}(p, q)u_n(q, E)\, dq \tag{3.11}$$

For a fixed E this equation shows that there are J open channels, where

$$\epsilon(J, 0) < E < \epsilon(J + 1, 0) \tag{3.12}$$

Other channels will be closed. Physically this means that in the asymptotic limit as $z \to \pm\infty$ there are only J discrete modes for the incoming and outgoing particles. However, because of the coupling to other modes, there can be additional localized modes in the center of the waveguide. Let us consider the specific case of $J = 1$, which is coupled to other partial waves. For $j = 1$, we have

$$u_1(p, E) = \delta[E - \epsilon(1, p)] - \frac{1}{2M(E - \epsilon(1, p))} \int_{-\infty}^{\infty} \Gamma_{11}(p - q) u_1(q, E)\, dq$$
$$- \frac{1}{2M(E - \epsilon(1, p))} \sum_{j>1} \int_{-\infty}^{\infty} \Gamma_{1j}(p, q) u_j(q, E)\, dq \tag{3.13}$$

and

$$(p^2 + \beta_j^2) u_j(p, E) = \sum_k \int_{-\infty}^{\infty} \Gamma_{jk}(p, q) u_k(q, E)\, dq, \qquad j > 1 \tag{3.14}$$

where

$$\beta_j^2 = (j^2\pi^2/L_a^2) - 2ME \tag{3.15}$$

Equations (3.13) and (3.14) are the single-particle wavefunctions in momentum space. To find an approximate solution to the set of coupled equations (3.13) and (3.14) we observe that $u_1(p, E)$ in the Born approximation can be written as

$$u_1(p, E) \approx \delta\{E - [\pi^2/(2ML_a^2)] - p^2/(2M)\} = \delta[(p^2 - \alpha^2)/2M] \tag{3.16}$$

where

$$\alpha^2 = 2M\{E - [\pi^2/(2ML_a^2)]\} \tag{3.17}$$

Substituting (3.16) in (3.14), we find

$$u_j(p, E) \approx [2M/(p^2 + \beta_j^2)][\Gamma_{j1}(p, \alpha) + \Gamma_{j1}(p, -\alpha)], \qquad j > 1 \tag{3.18}$$

From the definition of $\Gamma(p, q)$, equation (3.6), we obtain

$$u_j(p, E) \approx \frac{2M}{p^2 + \beta_j^2} \left\{ jB_{j1} \int_{-\infty}^{\infty} \cos(pz) \cos(\alpha z) \left(\frac{dL/dz}{L}\right)^2 dz \right.$$
$$- A_{j1} \left\{ \int_{-\infty}^{\infty} [(p^2 - \alpha^2 j) \cos(pz) \cos(\alpha z) \right.$$
$$\left. + p\alpha(j - 1) \sin(pz) \sin(\alpha z)] \ln\left(\frac{L(z)}{L_a}\right) dz \right\}, \qquad j > 1 \tag{3.19}$$

These integrals converge if $L(z)$ has the asymptotic behavior

$$\ln[L(z)/L_a] \to O[(1/z)^n], \qquad n \geq 2 \quad \text{as} \quad z \to \infty \tag{3.20}$$

If this is the case, then

$$[L^{-1}(dL/dz)]^2 \to O[(1/z)^{2n+1}], \qquad z \to \infty \tag{3.21}$$

and both integrals in (3.19) are finite. In general the second integral on the left side of (3.19) is the dominant term. Also note that for large integer j, $B_{1j} \approx 2(-1)^{j+1}(1/\pi j)^2$, $A_{1j} \approx (-1)^{j+1}/\pi j$, and $\beta_j^2 \approx j^2$; therefore the amplitude of $u_j(p, E)$ for large j is smaller by a factor of $(1/j)^2$. Thus only the first few modes, i.e., $j = 2, 3, \ldots$, are important and the others have negligible amplitudes.

As we mentioned earlier, the z dependence of the cross section of the waveguide is equivalent to the action of an external potential. This "fictitious" potential is nonseparable and depends on both y and z, but it does not couple the x degree of freedom with the y or z degrees of freedom. Denoting this external potential by $V(y, z)$, we can write the equation of motion for $a_j(p, t)$ in the following way:

$$i[da_j(p, t)/dt] = (1/2M)[p^2 + (j^2\pi^2/L_a^2)]a_j(p, t) + \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} \langle j, p \mid V \mid n, q\rangle a_n(q, t)\, dq = 0 \tag{3.22}$$

Comparing this with equation (3.5), we find

$$\langle j, p \mid V \mid n, q\rangle = (1/2M)\Gamma_{jn}(p, q) \tag{3.23}$$

This relation can be inverted to find the potential as a function of y and z. The results presented in this section are consistent with the findings of Andrews and Savage (1994). Using a coordinate transformation, these authors show that the motion of a particle in a nonuniform waveguide is equivalent to the motion of the same particle in a uniform waveguide but subject to a potential proportional to the eigenvalue. Here we have found a nonlocal potential which is equivalent to a local but energy- or velocity-dependent potential (Mott and Massey 1971).

4. AN EXAMPLE OF LOCALIZED MODES

Let us consider a waveguide where the cross section $2L(z)$ is given by

$$2L(z) = 2\exp[5\exp(-z^2/2)] \tag{4.1}$$

Here $L_a = 1$, and the cross sections at both ends are the same. If the energy of each of the incident particles is in the range

$$(\pi^2/2M) < E < (2\pi^2/M) \tag{4.2}$$

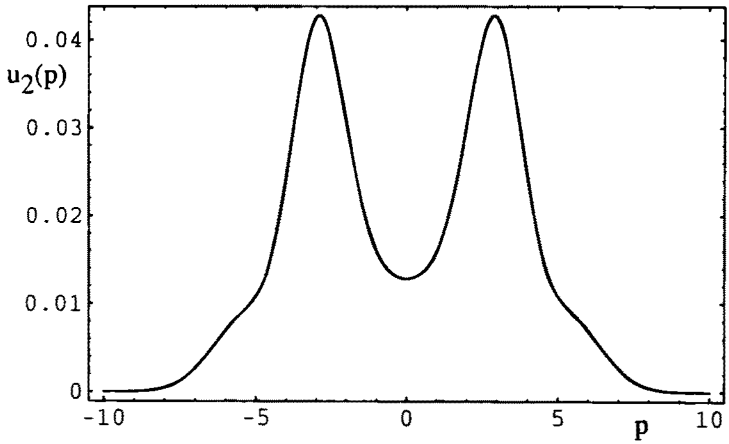

Fig. 1. Momentum-space wavefunction for the localized excitation in the waveguide $u_2(p)$ plotted as a function of p.

then according to (3.12) only one channel is open. In our calculation we have chosen

$$E = \pi^2/M \tag{4.3}$$

Then $\alpha = \pi$ and $\beta_j^2 = (j^2 - 2)\pi^2$ for $j > 1$. Since

$$\epsilon(1, 0) < E < \epsilon(2, 0) \tag{4.4}$$

only one transverse mode $j = 1$ will be entering and leaving the waveguide.

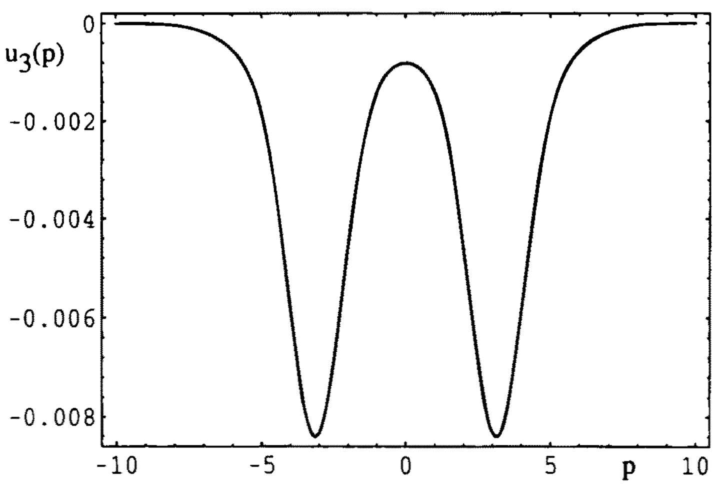

Fig. 2. Same as in Fig. 1, but for $u_3(p)$. Note that the amplitude of this wavefunction is smaller than $u_2(p)$.

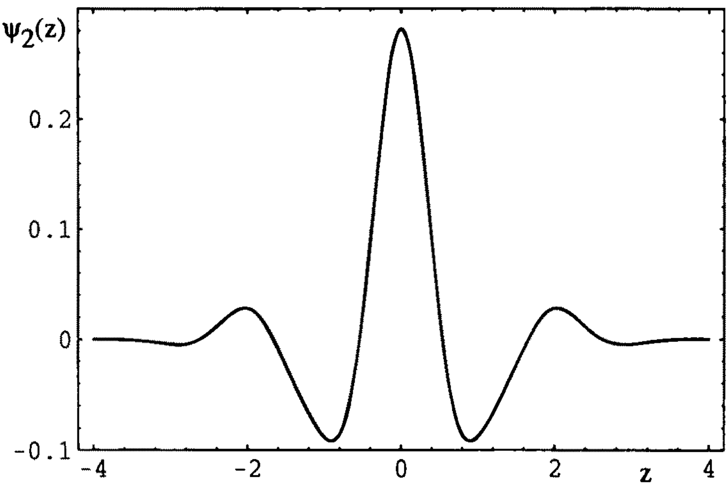

Fig. 3. The wavefunction $\psi_2(z)$, which is the Fourier transform of $u_2(p)$, shown as a function of z. This figure shows that the wavefunction is localized in the region where the cross section has a bulge.

From (3.19) we find $u_2(p)$ and $u_3(p)$ as functions of p. These are shown in Figs. 1 and 2. Both $u_2(p)$ and $u_3(p)$ have their maxima about $p = \pm\pi$, or for $p \approx \pm\alpha$, where α^2/M is the energy E of the incoming particle. This seems to be the property of all of the localized modes $u_j(p)$. The wavefunction in coordinate space is obtained from the Fourier transform of $u_j(p)$. Since

$$u_j(p) = u_j(-p) \tag{4.5}$$

then

$$\psi_j(z) = N_j \int_0^\infty u_j(p) \cos(pz)\, dp \tag{4.6}$$

where N_j is the normalization constant. The approximate wavefunction (not normalized) $\psi_2(z)$ found from the approximate $u_2(p)$ is shown in Fig. 3. The z coordinate of the peak of this wavefunction coincides with the z value of the maximum cross section, and the wavefunction is localized within the bulge of the waveguide.

5. CONCLUDING REMARKS

In this paper we have shown how the formalism of second quantization can be applied to study the motion of bosons in a waveguide with variable cross section. Exactly the same method can be used to discuss the flow of noninteracting fermions where similar equations are found. Another extension of this work is to the problem of determination of the propagating modes in a waveguide where the cross sections at the two ends are finite but unequal, i.e., $L(-\infty) \neq L(\infty)$ (Szafer and Stone, 1989). For this case we observe that the last term in (2.7) must be replaced by

$$i \sum_{n=0}^{\infty} \sum_{j=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dq\, dp(qn + pj)A_{jn}M(p - q)a_{jm}^{*}(q, t)a_{nm}(p, t)$$

where

$$M(p) = \int_{-\infty}^{\infty} dz \exp(ipz) [(dL/dz)/L] \tag{5.1}$$

Again assuming that $L(z)$ tends to finite values as $z \to -\infty$ or $z \to \infty$, then $[(dL/dz)/L]$ tends to zero at these limits, and if the rate of decrease of this quantity is fast enough so that (5.1) converges, then we have an equation of motion for the annihilation operator similar to (3.5).

One of the advantages of the present formulation is that the resulting solutions reflect the symmetry of the problem. For instance, if $L(z) = L(-z)$, as in the example of Section 4, then the localized modes are all symmetric (Figs. 1–3). Now in the coordinate-space formulation of the one-particle sector which is described by the Schrödinger equation, one encounters stiff differential equations (Razavy, 1994). Due to the accumulation of the numerical and roundoff errors of these equations the solution is not perfectly symmetric about $z = 0$. In addition, one can easily generalize the method presented here to the cases where the particles interact with each other as well as possibly interact with an external field.

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