Effective Lagrangian for quantum waveguides

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(Received 10 September 1997; revised manuscript received 29 December 1997)

Quantum mechanics of a particle living in a two-dimensional channel is studied using Feynman's path integration technique. Integrating out the transversal mode, we obtain the effective Lagrangian for motion along the center curve of the channel. Departure from free-particle dynamics takes place as the particle velocity increases towards a characteristic value that depends on curvature and width of the channel. Implications for mesoscopic normal metal rings are considered. [S0163-1829(98)05123-6]

Motivated by recent advances in microelectronics, Exner and Šeba[1,2] investigated the problem of Schrödinger dynamics in curved two-dimensional channels. Subsequently, Goldstone and Jaffe[3] considered a generalization to three-dimensional twisting tubes. In Ref. 1, the wave equation, subject to Dirichlet boundary conditions, is rewritten in natural curvilinear coordinates given by the intrinsic coordinates s of the reference (guiding) curve and the coordinate u along the normal to this curve (see Fig. 1). After a proper rescaling of the wave function, the Schrödinger equation acquires a negative effective potential proportional to the square of the curvature (of the reference curve). This kind of potential was found previously by several other authors,[4–7] but the possibility of observing the bound states and resonances in quantum wires[2] led to resurgence of interest in this problem. Moreover, as proposed recently by Bouchaud,[8] this curvature-induced potential may be even responsible for a Peierls-like transition of a superconducting vortex line to a folded state.

In the present paper, we study the quantum mechanics of a particle confined to the two-dimensional channel using Feynman's path integration method.[9–11] Our goal is to derive an effective Lagrangian describing the propagation along the reference curve of the channel. Though the transformed Hamiltonian used in this calculation agrees with that of Ref. 1, the effective Lagrangian is found to contain an additional term that is of fourth order in the velocity ds/dt. This term is due to the presence of the Jacobian [of the transformation $(x,y)\rightarrow(s,u)$] in the kinetic-energy operator. This induces a coupling term in the Lagrangian of the form $u\gamma(s)(ds/dt)^2$ where $\gamma(s)$ is the curvature. Integrating out the transverse degree of freedom u yields an effective Lagrangian containing not only the curvature-induced attractive potential but also a quartic term in the particle velocity that is likewise second order in the curvature. The physical significance of this term is that the effective mass of the quantum particle becomes velocity dependent as soon as the particle enters a curved portion of the waveguide. As a result, the momentum dependence of particle velocity departs from the linear, free-particle relation. The departure becomes significant when the velocity approaches a characteristic value that depends on the curvature and width of the waveguide. This result may have applications to mesoscopic normal metal rings, where typical values of the characteristic velocity that are below the bulk Fermi velocity are possible.

We consider a curved planar strip of fixed width. Adopting the notation of Ref. 1, the points in the strip are parametrized by

$$x=a(s)-ub'(s),$$

$$y=b(s)+ua'(s), \tag{1}$$

where primes indicate derivatives with respect to s. In distinction from Ref. 1, the reference curve $\Gamma\{a(s),b(s)\}$ is chosen to run through the center of the strip. Hence, the Dirichlet boundary conditions correspond to infinitely hard walls located at $u=\pm d/2$ (see Fig. 1). The transformation (1) implies that the metric tensor for the (s,u) coordinates is diagonal, with the components $g_{ss}=(1+u\gamma)^2$ and $g_{uu}=1$, where $\gamma(s)=[(a'')^2+(b'')^2]^{1/2}$ is the curvature. The Jacobian of the transformation (1) is $J=1+u\gamma(s)$.

The effective Lagrangian can be derived by considering the partition function

$$Z=\int d^2x\ \rho(\mathbf{x},\mathbf{x}), \tag{2}$$

where $\rho(\mathbf{x}',\mathbf{x})$ is the density matrix for a free particle in the coordinate representation[9]

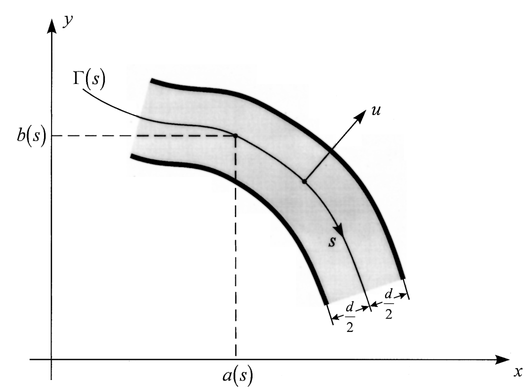

FIG. 1. A two-dimensional channel of width d with the reference curve $\Gamma(s)$.

$$\rho(\mathbf{x}',\mathbf{x}) = \langle \mathbf{x}'|e^{-\beta H}|\mathbf{x}\rangle = \int_{\mathbf{x}(0)}^{\mathbf{x}'(\hbar\beta)} \mathcal{D}_c \mathbf{x}(\tau) \times \exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m}{2}\dot{x}^2 d\tau \right), \tag{3}$$

where $H = -(\hbar^2/2m)\nabla^2$, and $\int \mathcal{D}_c \mathbf{x}(\tau)$ signifies path integration with the constraint that all the paths are confined to the strip.

Let us now consider the change of variables from (x,y) to (s,u) in the integral (2). With the use of Eq. (3), we obtain

$$Z = \int d^2q\; J\langle \mathbf{x}(\mathbf{q})|e^{-\beta\tilde{H}}|\mathbf{x}(\mathbf{q})\rangle, \tag{4}$$

where $\mathbf{q}$ is a shorthand for the coordinates (s,u), and $\tilde{H}$ is the free-particle Hamilton operator in terms of the coordinates (s,u),

$$\tilde{H} = -\frac{\hbar^2}{2m}\left[\frac{1}{J}\frac{\partial}{\partial s}\left(\frac{1}{J}\frac{\partial}{\partial s}\right) + \frac{1}{J}\frac{\partial}{\partial u}\left(J\frac{\partial}{\partial u}\right)\right]. \tag{5}$$

In the $\mathbf{q}$ representation, it is convenient to eliminate the Jacobian from the volume element in Eq. (4). This is achieved by introducing the rescaled wave functions[10]

$$\langle \mathbf{x}(\mathbf{q})|\alpha\rangle = J^{-1/2}\langle \mathbf{q}|\alpha\rangle, \tag{6}$$

where $|\alpha\rangle$ are the energy eigenstates. Using this relation, the partition function (4) takes the form

$$Z = \int d^2q \langle \mathbf{q}|e^{-\beta\bar{H}}|\mathbf{q}\rangle, \tag{7}$$

where the operator $\bar{H}$ is given by

$$\bar{H} = J^{1/2}\tilde{H}J^{-1/2} = -\frac{\hbar^2}{2m}\left[\frac{\partial}{\partial s}(1+u\gamma)^{-2}\frac{\partial}{\partial s} + \frac{\partial^2}{\partial u^2}\right] + V(s,u). \tag{8}$$

$V(s,u)$ is the curvature-induced attractive potential [see Eq. (3.1b) of Ref. 1]. For small and weakly varying $\gamma(s)$, we can approximate $V(s,u)$ by[1–3]

$$V(s) = -\frac{\hbar^2}{8m}\gamma^2(s). \tag{9}$$

According to Eq. (7), the Hamiltonian (8) guarantees a proper normalization of the density matrix $\rho(\mathbf{q},\mathbf{q})$. This should be compared with Ref. 1 where the same Hamiltonian is obtained by requiring the wave function to be normalized on the strip.

We now turn to the evaluation of $\rho(\mathbf{q}',\mathbf{q})$ using Feynman's path integral method. To facilitate the derivations, we replace the first term in square brackets of Eq. (8) by $(1+u\gamma)^{-2}\partial^2/\partial s^2$. This approximation is justified for weakly varying curvatures and it is exactly valid for mesoscopic rings where $\gamma' = 0$. Applying Feynman's time-slicing procedure, we obtain[9]

$$\rho(\mathbf{q}',\mathbf{q}) = \int_{\mathbf{q}(0)}^{\mathbf{q}'(\hbar\beta)} \mathcal{D}_c\mathbf{q}(\tau)\exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} L[\mathbf{q}(\tau),\dot{\mathbf{q}}(\tau)]d\tau\right\}, \tag{10}$$

where $L[\mathbf{q},\dot{\mathbf{q}}]$ is the Lagrangian in imaginary-time formulation. In terms of the (s,u) variables, we have

$$L[\mathbf{q},\dot{\mathbf{q}}] = \tfrac{1}{2}(1+u\gamma)^2 m\dot{s}^2 + \tfrac{1}{2}m\dot{u}^2 + V(s). \tag{11}$$

Using Eqs. (10) and (11), the partition function (7) becomes

$$Z = \int_{-\infty}^{\infty} ds \int_s^s \mathcal{D}s(\tau)\exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta}\left[\frac{1}{2}m\dot{s}^2 + V\right]d\tau\right\} \times \int_{-\infty}^{\infty} du F[s,\dot{s},u,u], \tag{12}$$

where

$$F[s,\dot{s},u,u] = \int_u^u \mathcal{D}_c u(\tau)\exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta}[\tfrac{1}{2}m\dot{u}^2 + m\gamma u\dot{s}^2 + \tfrac{1}{2}m\gamma^2\dot{s}^2u^2]d\tau\right\}. \tag{13}$$

The paths $u(\tau)$ involved in this path integral are constrained to the interval $(-d/2,d/2)$ imposed by the Dirichlet boundary condition. Defining the effective action for the motion along the coordinate s by

$$Z = \int_{-\infty}^{\infty} ds \int_s^s \mathcal{D}s(\tau)\exp\left(-\frac{1}{\hbar}S_{\text{eff}}\right), \tag{14}$$

we obtain with the use of Eq. (12)

$$S_{\text{eff}} = \int_0^{\hbar\beta} d\tau[\tfrac{1}{2}m\dot{s}^2 + V(s)] - \hbar\ \ln\int_{-\infty}^{\infty} du\; F[s,\dot{s},u,u]. \tag{15}$$

To simplify the evaluation of the last term in Eq. (15), we replace the infinite square-well potential by the harmonic oscillator potential $\frac{1}{2}m\omega^2u^2$ (Gaussian approximation). We also discard the last term in the exponent of Eq. (13), since it leads to a small enhancement of the mass. Thus, Eq. (13) reduces to

$$F_0[s,\dot{s},u,u] = \int_u^u \mathcal{D}u(\tau)\exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta}[\tfrac{1}{2}m\dot{u}^2 + \tfrac{1}{2}m\omega^2u^2 + m\gamma\dot{s}^2u]d\tau\right\}. \tag{16}$$

This is the path integral for a harmonic oscillator driven by the force $K(\tau) = m\gamma\dot{s}^2(\tau)$. With the use of Ref. 9, we obtain

$$\int_{-\infty}^{\infty} du\ F_0[s,\dot{s},u,u] = \frac{1}{2\sinh(\hbar\beta\omega/2)} \exp\left[\frac{1}{4m\omega\hbar}\int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\tau' e^{-\omega|\tau-\tau'|} K(\tau)K(\tau')\right]. \tag{17}$$

Introducing this result into Eq. (15), the effective Lagrangian for the motion along s becomes in the limit $T \to 0$,

$$L_{\mathrm{eff}}[s,\dot{s}] \simeq \tfrac{1}{2} m\dot{s}^2(\tau) + \frac{\hbar\omega}{2} + V(s) - \frac{m\gamma^2\dot{s}^2(\tau)}{4\omega}\int_{-\infty}^{\infty} d\tau' e^{-\omega|\tau-\tau'|}\dot{s}^2(\tau'). \tag{18}$$

We note that the second term is the ground-state energy of the transverse motion (see Refs. 1–3). To match the properties of the waveguide, the frequency ω is chosen so that the ground-state expectation value of u^2 for the infinite square well matches that for the harmonic oscillator. This amounts to taking $\omega \approx 30\hbar/md^2$.

If the function $\dot{s}^2(\tau')$ changes slowly (in the neighborhood of τ) in comparison with the exponential function, the τ' integral in Eq. (18) can be evaluated by replacing the latter function by the δ function. A criterion for the validity of this approximation can be established by noting that the largest contribution to $\rho(s',s)$ is due to the paths satisfying the classical equation of motion. The velocity change, imparted to the particle by the force dV/ds over the time interval $2\omega^{-1}$ is, using Eq. (9), given by

$$\Delta\dot{s} = \frac{\hbar^2}{2m^2\omega}\,\gamma\,\frac{d\gamma}{ds} \approx \frac{\hbar d^2}{60m}\,\gamma\,\frac{d\gamma}{ds}. \tag{19}$$

Letting $\dot{s} = v$, the above criterion amounts to requiring that $\Delta v^2/v^2 \ll 1$. Using Eq. (19), this implies a condition for the particle velocity

$$v \gg \frac{\hbar d^2}{30m}\,\gamma\,\frac{d\gamma}{ds} = v_{\mathrm{min}}. \tag{20}$$

Let us apply this condition to a periodically modulated waveguide with amplitude δ and wavelength $2\pi/Q$ (see Ref. 8). The curvature $\gamma(s) = \delta Q^2 \cos(Qs)$ must be smaller than $1/d$. Thus, Eq. (20) implies

$$v_{\mathrm{min}} = \frac{\hbar d^2\delta^2 Q^5}{30m} \leq \left(\frac{Q}{30k_F}\right) v_F. \tag{21}$$

Since the Fermi wave vector is of order $10^8\ \mathrm{cm}^{-1}$, v_{min} can be much smaller than the Fermi velocity for a sufficiently long modulation wavelength $\lambda = 2\pi/Q$. For instance, taking $\lambda = 10^{-5}$ cm, Eq. (21) yields $v_{\mathrm{min}}/v_F \leq 2\times10^{-4}$. In the case of a mesoscopic ring, we have $d\gamma/ds = 0$ and the evaluation of Eq. (18) with use of the δ function is exact.

Assuming that the condition (20) is satisfied, the effective Lagrangian (18), rewritten in terms of the velocity $v = ds/dt$ (where $t = -i\tau$ is the real-time variable), takes the form

$$L_{\mathrm{eff}} \simeq \frac{1}{2}\,m\left(1 + \frac{v^2}{v_c^2}\right)v^2 - V(s) + \frac{\hbar\omega}{2}, \tag{22}$$

where v_c is a characteristic velocity of the quantum waveguide

$$v_c(s) = \frac{\omega}{\gamma} \approx \frac{30\hbar}{md^2\gamma}. \tag{23}$$

We see from Eq. (22) that the effective mass of a quantum particle propagating along the reference curve is an increasing function of the velocity squared. It should be noted, however, that the rate of the increase, $1/v_c^2$, is limited since the curvature $\gamma(s)$ must be less than $1/d$. This condition implies, in conjunction with Eq. (23), that $v_c(s) \gtrsim 30\hbar/md$. In the limiting case $\gamma = 1/d$, we obtain $v_c \geq 3\times10^7$ cm/s for an electron waveguide of width $d = 100$ Å.

The velocity dependence of the effective mass has interesting consequences for the dynamics. Defining the generalized momentum $p = \partial L_{\mathrm{eff}}/\partial v$, we obtain with the use of Eq. (22)

$$v/v_c + 2(v/v_c)^3 = p/p_c, \tag{24}$$

where $p_c = mv_c$. The dispersion law $v(p)$ obtained from this equation shows substantial deviation from the case of a free particle. Specifically, the velocity remains below the $v = p/m$ line for all values of p. For instance, taking $p = p_c$, yields $v \approx 0.6v_c$. As p increases well above p_c the linear term in Eq. (24) plays a lesser role and the dispersion law crosses over to $v/v_c = (p/2p_c)^{1/3}$. It should be pointed out, however, that these conclusions are only valid within the Gaussian approximation that was adopted in the evaluation of the path integral (13). This imposes a limit on the magnitude of v for which Eq. (22) holds. We can see how this limit arises by calculating the correction to the ground-state energy by ordinary perturbation theory starting from Eq. (8).

Expanding the kinetic-energy operator in this equation to first order in γ, the perturbing Hamiltonian is

$$\overline{H}_1 = (\hbar^2 u\gamma/m)\,\frac{\partial^2}{\partial s^2}. \tag{25}$$

The second-order energy correction obtained with $\overline{H}_1$ connecting the ground state ψ_1 to the next excited state ψ_2 is

$$\Delta E^{(2)} = -\frac{p^4}{2m^3 v_c^2}. \tag{26}$$

The same result is obtained by calculating the energy correction from the effective Lagrangian (18) using the method of the transition amplitude[11] with the assumption that the momentum p is a constant of motion. In the Gaussian approximation, there is no energy correction of higher order than second. This can be verified explicitly from the formula for the fourth-order correction

$$\Delta E^{(4)} = \frac{|\langle 1|\overline{H}_1|2\rangle|^2 |\langle 2|\overline{H}_1|3\rangle|^2}{(E_1-E_2)^2(E_1-E_3)} - \frac{|\langle 1|\overline{H}_1|2\rangle|^4}{(E_1-E_2)^3}. \tag{27}$$

Assuming that the kets $|1\rangle$, $|2\rangle$, and $|3\rangle$ are the lowest eigenstates of a harmonic oscillator, the two terms on the right-hand side of Eq. (27) exactly cancel. This is to be expected since the perturbation H_1 is linear in the displacement u so that we are dealing with the case of a forced harmonic oscillator that is solved exactly by the second-order perturbation theory.[11]

For the infinite square well, the fourth-order correction to the energy is, however, nonzero. Its magnitude provides us with a criterion of validity of the Gaussian result (22). With the eigenstates for the well, Eq. (27) yields

$$\Delta E^{(4)} \approx \frac{2.2p^8}{d^2\gamma^2 m^7 v_c^6}. \tag{28}$$

From Eqs. (26) and (28) it follows that the magnitudes of $\Delta E^{(2)}$ and $\Delta E^{(4)}$ are equal when $p/p_c \approx 0.7(d\gamma)^{1/2}$. This means that the Gaussian approximation, leading to Eq. (22), is valid only for momenta $p \ll p_c$. For real electron waveguides, the potential well is never infinite being determined by the work function of the sample. Thus, the restriction on the momenta for a finite well is probably less severe as the fourth-order energy correction is smaller than that for the infinite well.

According to Büttiker, Imry, and Landauer,[12] a normal metal ring threaded by a magnetic flux should carry a persistent current. The magnitude of this current is of order ev_F/L, where L is the circumference of the ring, as it is mostly contributed by the electrons in the highest occupied levels near E_F. In this region the electron energy spectrum is expected to be modified by the quartic term in Eq. (22). In view of Eq. (23), as soon as v_c drops below the bulk Fermi velocity the persistent current develops a dependence upon the width d of the ring. Since disorder tends to compete with the curvature-induced transverse excitations, the width should not exceed the mean free path of the ring.

In summary, we find that quantum dynamics in a curved channel is influenced by excitations of the transverse modes. Integrating out these modes, we obtain an effective Lagrangian for the motion along the reference curve of the channel. Within the Gaussian approximation, this Lagrangian contains a term that is quartic in particle velocity. Consequently, the linear dependence of the velocity upon the particle momentum is modified as the momentum approaches a critical value that is a function of the curvature and width of the waveguide. For Dirichlet boundary conditions, the departure from the Gassian approximation is discussed using perturbation theory for the ground-state energy. Similar conclusions can be drawn for three-dimensional twisting tubes with the Dirichlet boundary condition since the coupling to transverse coordinates is also present in their Hamiltonian.[3]

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