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Wavefunction, energy spectrum and uncertainty relation for a particle contained between moving potential walls

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Abstract. The temporal energy spectrum $E^{s,a}(t)$ and the uncertainty product $\Delta p^{s,a}(t)\Delta x^{s,a}(t)$ are derived from an analytical solution $\psi(x, t)$ of the initial-boundary-value problem for the Schrödinger equation of a particle contained between moving potential walls at $x = \pm s(t)$, which are set in motion according to an arbitrary (non-relativistic) translation $s = s(t)$ at time $t = 0$. Both symmetrical (s) and antisymmetrical (a) particle states are considered as initial conditions in the region $-s(0) \leq x \leq +s(0)$. The physical implications of the compression and expansion of the probability density by the moving walls on the wave mechanics of the particle are discussed. The results are understandable within the statistical interpretation of quantum theory.

1. Introduction

Solutions of the time-dependent Schrödinger equation are not only of physical importance in view of the peculiarities this parabolic equation exhibits in time-dependent situations (Husumi 1953, Lewis and Riesenfeld 1969, Stutz and Schlitt 1970, Borghese *et al* 1974, Wilhelm and Hong 1980), but also of theoretical interest due to the obvious mathematical difficulties. Exact (non-perturbation) analytical solutions of the Schrödinger equation with moving boundary conditions have not apparently been achieved previously. For these reasons, we treat the simple, but fundamental, initial-boundary-value problem for the wavefunction $\psi(x, t)$ of a particle, which is contained between infinite potential walls $U = \infty$ at $x = \pm s(t)$. These 'walls' are initially at $x = \pm s(0) = \pm a$, and are set in motion at time $t = 0$ according to a non-relativistic ($|\dot{s}(t)| \ll c$), but otherwise arbitrary, translation law $s = s(t)$. Both expansion ($\dot{s}(t) > 0$) and contraction ($\dot{s}(t) < 0$) of the 'box' are considered.

The problem under consideration can be treated both by Laplace transformation and finite integral transformation for arbitrary wall motions $s(t)$ (Wilhelm 1982). These methods lead, however, to complicated integral equations which do not appear to be solvable in closed form (Wilhelm 1982). Furthermore, the moving-boundary-value problem for the Schrödinger equation can be dealt with by group theory in the case of special wall motions $s(t)$. The latter approach is frequently used for the solution of nonlinear partial differential equations (e.g. gas dynamics (Liron and Wilhelm 1975), plasma dynamics (Wilhelm 1973), and hydrodynamic quantum mechanics (Janossy and Ziegler 1963)). For these reasons, the initial-boundary-value problem for the one-particle Schrödinger equation with two moving potential walls at $x = \pm s(t)$ is solved herein by an extended Fourier method with x- and t-dependent eigenfunctions, which results in elegant analytical solutions. The time dependence of the eigenfunctions considers the temporal change of the region $-s(t) \leqslant x \leqslant +s(t)$ in which the spatial (x) Fourier series expansion is carried through. As initial conditions, the known symmetrical and antisymmetrical wavefunctions of the particle in the undeformed box $-a \leqslant x \leqslant +a$ are chosen.

The method of x- and t-dependent eigenfunctions reduces the mathematical problem under consideration to an infinite system of coupled first-order differential equations with variable coefficients for the Fourier amplitudes $\psi_k(t)$ of the wavefunction $\psi(x, t)$. This system is transformed to coupled Volterra integral equations by integration, which are solved by analytical methods for the functions $\psi_k(t)$. Thus, exact Fourier series solutions are obtained for the wavefunction $\psi(x, t)$ of the particle in the box with moving walls. From the latter, analytical formulae for the time-dependent energy spectrum and uncertainty relation of the particle are deduced. The effects of wall motion on the quantum dynamics of the particle are discussed.

2. Initial-boundary-value problem

The temporal development of the (non-relativistic) wavefunction $\psi(x, t)$ of a particle m contained in the well between two infinite potential walls $U = \infty$ at $x = \pm s(t = 0) = \pm a$ (figure 1), which are set into motion at time $t = 0$ according to an arbitrary translation law $s(t)$, is determined by the initial-boundary-value problem for the Schrödinger equation with moving boundary conditions:

$$\partial\psi/\partial t = \mathrm{i}(\hbar/2m)\,\partial^2\psi/\partial x^2 \qquad -s(t) < x < +s(t) \qquad 0 < t < \hat{t} \tag{1}$$

$$\psi(x, t = 0) = \psi_0(x) \qquad -a < x < +a \tag{2}$$

$$\psi(x = \pm s(t), t) = 0 \qquad 0 < t < \hat{t} \tag{3}$$

where

$$s(t = 0) = a. \tag{4}$$

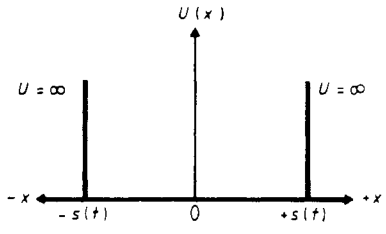

Figure 1. One-dimensional box with moving potential walls $U = \infty$ at $x = \pm s(t)$.

The function $s(t)$ is related to the speeds $v_\pm(t) = \pm\,\mathrm{d}s(t)\,\mathrm{d}t$ of the walls at $x = \pm s(t)$ by

$$s(t) = a \pm \int_0^t v_\pm(t')\,\mathrm{d}t' \qquad 0 \leqslant t < \hat{t} \tag{5}$$

where

$$0 \leqslant s(t) \leqslant a \qquad s(t = \hat{t}) = 0 \qquad 0 < \hat{t} < \infty \tag{6}$$

or

$$a < s(t) < \infty \qquad s(t=\hat{t}) < \infty \qquad 0 < \hat{t} < \infty \tag{7}$$

depending on whether the potential walls at $x = \pm s(t)$ move towards (equation (6)) or away from (equation (7)) each other. Since the Schrödinger equation is non-relativistic, the wall speeds are assumed to be small compared with the speed of light, $|v_\pm(t)| \ll c$. Otherwise, $s(t)$ and $v_\pm(t)$ are arbitrary, physically well behaved functions of time.

The initial condition (2) is a normalisable function $\psi_0(x)$, which is compatible with the uncertainty principle for the particle in the box $-a < x < +a$. We take for $\psi_0(x)$ any one of the symmetrical (s) or antisymmetrical (a) normalised eigenfunctions of the box particle m in the nth energy state $E_n^{s,a}(0) = (\pi^2\hbar^2/8ma^2)n^2$ (Schiff 1955):

$$\psi_0^{s}(x) = a^{-1/2}\cos(n\pi x/2a) \qquad -a < x < +a \qquad n = 1, 3, 5, \ldots \tag{8}$$

$$\psi_0^{a}(x) = a^{-1/2}\sin(n\pi x/2a) \qquad -a < x < +a \qquad n = 2, 4, 6, \ldots. \tag{9}$$

The initial normalisation $\int_{-a}^{+a}\psi_0(x)^2\,dx = 1$ of the complex wavefunction $\psi(x,t)$ remains conserved for $t > 0$, since the probability density $\rho(x,t) = \psi(x,t)^*\psi(x,t)$ is conserved for the boundary conditions (3). The symmetric and antisymmetric initial conditions (equations (8) and (9) respectively) for the states n give, for the particle in the box $-a \leqslant x \leqslant +a$, an initial momentum uncertainty

$$\pm\Delta p^{s,a}(0) = \pm\hbar(n\pi/2a) \qquad n = \begin{cases} 1, 3, 5, \ldots \\ 2, 4, 6, \ldots \end{cases}. \tag{10}$$

3. Analytical solutions

For the symmetric (s) and antisymmetric (a) initial conditions (8) and (9), the solutions $\psi(x,t)$ of the initial-boundary-value problem (1)–(3) with homogeneous boundary conditions are necessarily symmetric and antisymmetric respectively. In the absence of boundary motion, $s(t) = a$, the eigenfunctions of equation (1) would be

$$f_k^{s,a}(x) = \begin{matrix}\cos\\ \sin\end{matrix}\left(k\frac{\pi}{2}\frac{x}{a}\right)\Big/ a^{1/2}.$$

For these reasons, we choose the normalised eigenfunctions of equation (1) for the variable region $-s(t) \leqslant x \leqslant +s(t)$ as

$$f_k^{s,a}(x,t) = s(t)^{-1/2}\begin{matrix}\cos\\ \sin\end{matrix}\left(k\frac{\pi}{2}\frac{x}{s(t)}\right) \qquad k = \begin{cases} 1, 3, 5, \ldots \\ 2, 4, 6, \ldots \end{cases} \tag{11}$$

where the eigenvalues k are determined by the homogeneous boundary conditions (3). The orthogonality relations for the x- and t-dependent eigenfunctions are

$$\int_{-s(t)}^{+s(t)} f_k^{s,a}(x,t) f_j^{s,a}(x,t)\,dx = \delta_{kj} \qquad \delta_{kj} = \begin{cases} 1 & k = j \\ 0 & k \neq j \end{cases}. \tag{12}$$

Any symmetric (s) or antisymmetric (a) solution $\psi(x,t)$ of equations (1)–(3) can be represented by the expansion in orthogonal eigenfunctions:

$$\psi^{s,a}(x,t) = \sum_k \psi_k^{s,a}(t) f_k^{s,a}(x,t) \tag{13}$$

where

$$\psi_k^{s,a}(t)=\int_{-s(t)}^{+s(t)}\psi^{s,a}(x,t)f_k^{s,a}(x,t)\,dx \tag{14}$$

are the Fourier amplitudes (by equation (12)). Equations (11)–(14) extend Fourier's theorem to series expansions in time-dependent regions $-s(t)\leqslant x\leqslant +s(t)$.

The Fourier amplitudes $\psi_k^{s,a}(t)$ are determined by differential equations, which are obtained by multiplication of equation (1) with $f_k^{s,a}(x,t)$ and integration over the variable region $-s(t)\leqslant x\leqslant +s(t)$:

$$\int_{-s(t)}^{+s(t)}\frac{\partial\psi}{\partial t}f_k^{s,a}\,dx=\frac{i\hbar}{2m}\int_{-s(t)}^{+s(t)}\frac{\partial^2\psi}{\partial x^2}f_k^{s,a}\,dx \tag{15}$$

where

$$\int_{-s(t)}^{+s(t)}\frac{\partial^2\psi}{\partial x^2}f_k^{s,a}\,dx=\left[f_k^{s,a}\frac{\partial\psi}{\partial x}-\frac{\partial f_k^{s,a}}{\partial x}\psi\right]_{-s(t)}^{+s(t)}+\int_{-s(t)}^{+s(t)}\psi\frac{\partial^2 f_k^{s,a}}{\partial x^2}\,dx \tag{16}$$

$$\int_{-s(t)}^{+s(t)}\frac{\partial\psi}{\partial t}f_k^{s,a}\,dx=\frac{d}{dt}\int_{-s(t)}^{+s(t)}\psi f_k^{s,a}\,dx-\int_{-s(t)}^{+s(t)}\psi\frac{\partial f_k^{s,a}}{\partial t}\,dx-\dot{s}(t)[\psi f_k^{s,a}]_{-s(t)}^{+s(t)} \tag{17}$$

and

$$\int_{-s(t)}^{+s(t)}\psi\frac{\partial f_k^{s,a}}{\partial t}\,dx=-\frac{1}{2}\frac{\dot{s}(t)}{s(t)}\psi_k^{s,a}(t)+\frac{\dot{s}(t)}{s(t)}\sum_j C_{kj}^{s,a}\psi_j^{s,a}(t) \tag{18}$$

with

$$C_{kj}^{s,a}=\pm\frac{2}{\pi}k\int_{-\pi/2}^{+\pi/2}\xi\,{}^{\cos}_{\sin}(j\xi)\,{}^{\sin}_{\cos}(k\xi)\,d\xi \tag{19}$$

for $k=j$ and $k\neq j$ ($j,k=1,3,5,\ldots$ (s) or $j,k=2,4,6,\ldots$ (a)). In particular,

$$C_{kj}^{s,a}=1/2=C_{jk}^{s,a}\qquad j=k \tag{20}$$

$$C_{kj}^{s,a}=\mp k\left(\frac{\cos(k+j)\pi/2}{k+j}\pm\frac{\cos(k-j)\pi/2}{k-j}\right)=-C_{jk}^{s,a}\qquad j\neq k \tag{21}$$

where $\cos(k\pm j)\pi/2=(-1)^{(k\pm j)/2}$. In view of the boundary conditions (3), the square brackets in equations (16) and (17) vanish. By using equations (11) and (14) the integral (16) reduces to $-(k\pi/2s(t))^2\psi_k^{s,a}(t)$.

According to equations (15)–(18), the Fourier amplitudes of the symmetrical (s) and antisymmetrical (a) solutions satisfy the initial-value problem

$$\frac{d\psi_k^{s,a}}{dt}+\frac{i\hbar}{2m}\left(\frac{k\pi}{2s(t)}\right)^2\psi_k^{s,a}=\frac{\dot{s}(t)}{s(t)}\sum_{j\neq k}C_{kj}^{s,a}\psi_j^{s,a} \tag{22}$$

$$\psi_k^{s,a}(t=0)=\delta_{kn} \tag{23}$$

for coupled differential equations of first order. By equations (8), (9) and (14) all initial values with $k\neq n$ vanish but $\psi_n^{s,a}(t=0)=1$. The subsequent transformations (with integrating factor)

$$\Psi_k^{s,a}(t)=\exp\left(\frac{i\hbar}{2m}\left(\frac{k\pi}{2}\right)^2\int_0^t\frac{dt'}{s(t')^2}\right)\psi_k^{s,a}(t) \tag{24}$$

and

$$\tau = \ln(s(t)/a) \leqslant 0 \qquad s(t) \leqslant a \qquad \Psi_k^{s,a}(\tau) \equiv \Psi_k^{s,a}(t) \tag{25}$$

reduce equations (22) and (23) to the simpler initial-value problem with variable coefficients:

$$\mathrm{d}\Psi_k^{s,a}/\mathrm{d}\tau = \sum_{j\neq k} C_{kj}^{s,a} \exp[\mathrm{i}\omega(\tau)(k^2-j^2)]\Psi_j^{s,a} \tag{26}$$

$$\Psi_k^{s,a}(\tau=0) = \delta_{kn} \tag{27}$$

where

$$\omega(\tau) = (\hbar/2m)(\pi/2)^2 \int_0^{t(\tau)} s(t)^{-2}\,\mathrm{d}t \tag{28}$$

and $t(\tau)$ is given by inversion of the known function $s(t) = a\mathrm{e}^{\tau}$, equation (25). Since $k = 1, 3, 5, \ldots$ for the symmetric (s) and $k = 2, 4, 6, \ldots$ for the antisymmetric (a) solutions $\psi(x, t)$, the matrices $\mathbf{C}^{s,a}$ in equation (26) are of the form

$$\mathbf{C}^{s} = \lim_{\nu\to\infty} \begin{pmatrix} 0 & C_{13}^{s} & C_{15}^{s} & \ldots & C_{1\nu}^{s} \\ C_{31}^{s} & 0 & C_{35}^{s} & \ldots & C_{3\nu} \\ \vdots & & & & \\ C_{\nu 1} & C_{\nu 3} & C_{\nu 5} & \ldots & 0 \end{pmatrix} \tag{29}$$

$$\mathbf{C}^{a} = \lim_{\nu\to\infty} \begin{pmatrix} 0 & C_{24}^{a} & C_{26}^{a} & \ldots & C_{2\nu}^{a} \\ C_{42}^{a} & 0 & C_{46}^{a} & \ldots & C_{4\nu}^{a} \\ \vdots & & & & \\ C_{\nu 2}^{a} & C_{\nu 4}^{a} & C_{\nu 6}^{a} & \ldots & 0 \end{pmatrix} \tag{30}$$

where

$$C_{kj}^{s} = -k[(k-j)(-1)^{(k+j)/2} + (k+j)(-1)^{(k-j)/2}]/(k^2-j^2) = -C_{jk}^{s}$$
$$j; k = 1, 3, 5, \ldots \tag{31}$$

$$C_{kj}^{a} = -2(-1)^{(k+j)/2} kj/(k^2-j^2) = -C_{jk}^{a} \qquad j; k = 2, 4, 6, \ldots \tag{32}$$

by equation (21). Integration of equations (26) and (27) demonstrates that the initial-value problem is mathematically equivalent to the system of coupled Volterra integral equations

$$\Psi_k^{s,a}(\tau) = \delta_{kn} + \sum_{j\neq k} C_{kj}^{s,a} \int_0^{\tau} \exp[\mathrm{i}\omega(\tau')(k^2-j^2)]\Psi_j^{s,a}(\tau')\,\mathrm{d}\tau'. \tag{33}$$

The method of successive approximations yields as solutions in the Nth approximation ($N = 0, 1, 2, \ldots$):

$$\Psi_{k(0)}^{s,a}(\tau) = \delta_{kn} \tag{34}$$

$$\Psi_{k(1)}^{s,a}(\tau) = \delta_{kn} + C_{kn}^{s,a} \int_0^{\tau} \exp[\mathrm{i}\omega(\tau_1)(k^2-n^2)]\,\mathrm{d}\tau_1 \tag{35}$$

$$\Psi^{s,a}_{k(2)}(\tau)=\delta_{kn}+C^{s,a}_{kn}\int_0^{\tau}\exp[i\omega(\tau_1)(k^2-n^2)]\,d\tau_1$$
$$+\sum_{j\neq k}C^{s,a}_{kj}C^{s,a}_{jn}\int_0^{\tau}\exp[i\omega(\tau_2)(k^2-j^2)]\,d\tau_2\int_0^{\tau_2}\exp[i\omega(\tau_1)(j^2-n^2)]\,d\tau_1 \tag{36}$$

$$\Psi^{s,a}_{k(3)}(\tau)=\delta_{kn}+C^{s,a}_{kn}\int_0^{\tau}\exp[i\omega(\tau_1)(k^2-n^2)]\,d\tau_1$$
$$+\sum_{j\neq k}C^{s,a}_{kj}C^{s,a}_{jn}\int_0^{\tau}\exp[i\omega(\tau_2)(k^2-j^2)]\,d\tau_2\int_0^{\tau_2}\exp[i\omega(\tau_1)(j^2-n^2)]\,d\tau_1$$
$$+\sum_{j\neq k}C^{s,a}_{kj}\sum_{i\neq j}C^{s,a}_{ji}C^{s,a}_{in}\int_0^{\tau}\exp[i\omega(\tau_3)(k^2-j^2)]\,d\tau_3$$
$$\times\int_0^{\tau_3}\exp[i\omega(\tau_2)(j^2-i^2)]\,d\tau_2\int_0^{\tau_2}\exp[i\omega(\tau_1)(i^2-n^2)]\,d\tau_1. \tag{37}$$

Hence, the solution in the Nth approximation is

$$\Psi^{s,a}_{k(N)}(\tau)=\delta_{kn}+C^{s,a}_{kn}T(\tau,kn)+\sum_{j\neq k}C^{s,a}_{kj}C^{s,a}_{jn}T(\tau,kjjn)$$
$$+\sum_{j\neq k}C^{s,a}_{kj}\sum_{i\neq j}C^{s,a}_{ji}C^{s,a}_{in}T(\tau,kjjiin)+\dots$$
$$+\sum_{j\neq k}C^{s,a}_{kj}\sum_{i\neq j}C^{s,a}_{ji}\sum_{l\neq j}C^{s,a}_{il}\dots\sum_{s\neq r}C_{rs}$$
$$\times\sum_{t\neq s}C^{s,a}_{st}C^{s,a}_{t\underline{n}}T(\tau,kjjiill\dots rrsstt\underline{n})\qquad(N-1\text{ sums}) \tag{38}$$

where

$$T(\tau,\underline{k}jjiill\dots rrsstt\underline{n})=\int_0^{\tau}d\tau_N\int_0^{\tau_N}d\tau_{N-1}\int_0^{\tau_{N-1}}d\tau_{N-2}\dots$$
$$\times\int_0^{\tau_4}d\tau_3\int_0^{\tau_3}d\tau_2\int_0^{\tau_2}d\tau_1\,\exp i[\omega(\tau_N)(\underline{k}^2-j^2)$$
$$+\omega(\tau_{N-1})(j^2-i^2)+\omega(\tau_{N-2})(i^2-l^2)+\dots$$
$$+\omega(\tau_3)(r^2-s^2)+\omega(\tau_2)(s^2-t^2)+\omega(\tau_1)(t^2-\underline{n}^2)] \tag{39}$$

is an N-fold integral, $N=1,2,3,\dots$. In the absence of the multiple integrals $T(\tau,\underline{k}\dots\underline{n})$, the multiple sums in equation (38) could be written as kn elements of the product of $N=0,1,2,\dots$ matrices **C** since

$$(\mathbf{C})^0_{kn}=\delta_{kn},\dots,(\mathbf{C})^N_{\underline{k}\underline{n}}=\sum_{j\neq k}C_{kj}\sum_{i\neq l}C_{ji}\sum_{l\neq j}C_{il}\dots\sum_{s\neq r}C_{rs}\sum_{t\neq s}C_{st}C_{t\underline{n}}\qquad(N-1\text{ sums}). \tag{40}$$

From the analytical solution (37) for $\Psi^{s,a}_k(\tau)$, the solution for $\Psi^{s,a}_k(t)$ is obtained as

$$\Psi^{s,a}_k(t)=\Psi^{s,a}_k(\tau=\ln(s(t)/a))\qquad t\geqslant 0. \tag{41}$$

According to equations (24) and (25), the corresponding solutions for the (complex) Fourier amplitudes are

$$\psi_k^{s,a}(t)=\Psi_k^{s,a}(t)\exp\left[-\frac{i\hbar}{2m}\left(\frac{k\pi}{2}\right)^2\int_0^t\frac{dt'}{s(t')^2}\right]. \tag{42}$$

Thus, we find the following Schrödinger fields $\psi^{s,a}(x,t)$ for the symmetric (s) and antisymmetric (a) initial conditions (8) and (9), which determine the quantum dynamics of the particle m in the contracting or expanding box:

$$\psi^{s,a}(x,t)=s(t)^{-1/2}\sum_k\Psi_k^{s,a}(t)\exp\left[-\frac{i\hbar}{2m}\left(\frac{k\pi}{2}\right)^2\int_0^t\frac{dt'}{s(t')^2}\right]\begin{matrix}\cos\\ \sin\end{matrix}\left(k\frac{\pi}{2}\frac{x}{s(t)}\right)$$
$$k=\begin{cases}1,3,5,\ldots\\ 2,4,6,\ldots.\end{cases} \tag{43}$$

The probability densities $\rho^{s,a}(x,t)=(\bar{\psi}(x,t)\psi(x,t))^{s,a}$ of the particle in the symmetric (s) and antisymmetric (a) box states are

$$\rho^{s,a}(x,t)=\frac{1}{s(t)}\sum_j\sum_k\bar{\Psi}_j^{s,a}(t)\Psi_k^{s,a}(t)\exp\left[-\frac{i\hbar}{2m}\left(\frac{\pi}{2}\right)^2(k^2-j^2)\int_0^t\frac{dt'}{s(t')^2}\right]$$
$$\times\begin{matrix}\cos\\ \sin\end{matrix}\left(j\frac{\pi}{2}\frac{x}{s(t)}\right)\begin{matrix}\cos\\ \sin\end{matrix}\left(k\frac{\pi}{2}\frac{x}{s(t)}\right)\qquad j,k=\begin{cases}1,3,5,\ldots\\ 2,4,6,\ldots.\end{cases} \tag{44}$$

Equations (43) and (44) reduce to the (s, a) wavefunctions and probability densities of the particle in the box with fixed walls for $s(t)=a$:

$$\psi^{s,a}(x,t)=a^{-1/2}\begin{matrix}\cos\\ \sin\end{matrix}\left(n\frac{\pi}{2}\frac{x}{a}\right)\exp\left[-\frac{i\hbar}{2m}\left(\frac{n\pi}{2a}\right)^2t\right]\qquad n=\begin{cases}1,3,5,\ldots\\ 2,4,6,\ldots\end{cases} \tag{45}$$

$$\rho^{s,a}(x,t)=a^{-1}\begin{matrix}\cos^2\\ \sin^2\end{matrix}\left(n\frac{\pi}{2}\frac{x}{a}\right)\qquad n=\begin{cases}1,3,5,\ldots\\ 2,4,6,\ldots\end{cases} \tag{46}$$

since $\Psi_k^{s,a}(t)=\delta_{kn}$ for $s(t)\to a(\tau\to 0)$ by equations (25), (38) and (39).

Since the matrices $(\mathbf{A}_{kj}(\tau))=(C_{kj}^{s,a}\exp[i\omega(\tau)(k^2-j^2)])$ and $(\mathbf{B}_{kj}(\tau))=\int_0^\tau(A_{kj}(\tau'))\,d\tau'$ do not commute, equation (26) probably has no closed-form solution. Stepanov (1963) has demonstrated that the successive approximations of linear systems of differential equations converge in $0<|\tau|<\infty$ for τ-dependent coefficients which are continuous in $0<|\tau|<\infty$. In the case of the system (33) with τ-dependent coefficient factors $F_{kj}(\tau)=\exp[i\omega(\tau)(k^2-j^2)]$, where $|F_{kj}(\tau)|=1$, the applicability of the method of successive approximations is obvious from the convergence of the solution of the system $\Psi_k(\tau)=\delta_{kn}+\sum_{j\neq k}C_{kj}\int_0^\tau\Psi_j(\tau')\,d\tau'$, which is $\Psi_k(\tau)=\exp(\mathbf{C}\tau)\Psi_k(0)$ (the multiple τ integrals of order $N=0,1,2,\ldots$ reduce for constant coefficients to $T(\tau,\underline{k}\ldots\underline{n})=\tau^N/N!$).

The analytical solution (38) is rather involved since multiple τ integrals have to be worked out for given functions $\omega(\tau)$ or $s(t)$, equation (28). For complicated translations $s(t)$, it is advisable to solve the initial-value problem (22) and (23) numerically.

4. Particle energy

Before the deformation of the box $-a \leqslant x \leqslant +a$ occurs, the particle has a (fixed) energy eigenvalue $E_n^{s,a}(0)$ in each of the symmetric (s) and antisymmetric (a) states n. According to the associated (s, a) wavefunctions (8) and (9)

$$E_n^{s,a}(0) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2 \qquad n = \begin{cases} 1, 3, 5, \ldots \\ 2, 4, 6, \ldots \end{cases} \tag{47}$$

These energy eigenvalues change with time when the walls of the box are moved. At any time $0 < t < \hat{t}$, the expectation value of the particle energy is

$$E_n^{s,a}(t) = \mathrm{i}\hbar \int_{-s(t)}^{+s(t)} \bar{\psi}^{s,a}(x, t) \frac{\partial \psi^{s,a}(x, t)}{\partial t} \, \mathrm{d}x \tag{48}$$

where

$$\bar{\psi}^{s,a}(x, t) = s(t)^{-1/2} \sum_k \bar{\psi}_k^{s,a}(t) \begin{matrix}\cos \\ \sin\end{matrix}\left(k \frac{\pi}{2} \frac{x}{s(t)}\right) \tag{49}$$

$$\begin{aligned} \frac{\partial \psi^{s,a}(x, t)}{\partial t} = &-\frac{1}{2} \frac{\dot{s}(t)}{s(t)} s(t)^{-1/2} \sum_k \psi_k^{s,a}(t) \begin{matrix}\cos \\ \sin\end{matrix}\left(k \frac{\pi}{2} \frac{x}{s(t)}\right) \\ &\pm \frac{\dot{s}(t)}{s(t)} s(t)^{-1/2} \sum_k k \frac{\pi}{2} \frac{x}{s(t)} \psi_k^{s,a}(t) \begin{matrix}\sin \\ \cos\end{matrix}\left(k \frac{\pi}{2} \frac{x}{s(t)}\right) \\ &+ s(t)^{-1/2} \sum_k \frac{\mathrm{d}\psi_k^{s,a}(t)}{\mathrm{d}t} \begin{matrix}\cos \\ \sin\end{matrix}\left(k \frac{\pi}{2} \frac{x}{s(t)}\right) \end{aligned} \tag{50}$$

with

$$\frac{\mathrm{d}\psi_k^{s,a}}{\mathrm{d}t} = -\frac{\mathrm{i}\hbar}{2m}\left(\frac{k\pi}{2s(t)}\right)^2 \psi_k^{s,a} + \frac{\dot{s}(t)}{s(t)} \sum_{j \neq k} C_{kj}^{s,a} \psi_j^{s,a} \tag{51}$$

by equations (43), (42) and (22). The terms in equation (50) yield, in the same sequence, the following contributions to the particle energy (48):

$$E_{n1}^{s,a}(t) = -\frac{\mathrm{i}\hbar}{2} \frac{\dot{s}(t)}{s(t)} \sum_k \bar{\psi}_k^{s,a}(t) \psi_k^{s,a}(t) \tag{52}$$

$$E_{n2}^{s,a}(t) = +\frac{\mathrm{i}\hbar}{2} \frac{\dot{s}(t)}{s(t)} \sum_k \bar{\psi}_k^{s,a}(t) \psi_k^{s,a}(t) + \mathrm{i}\hbar \frac{\dot{s}(t)}{s(t)} \sum_k \sum_{j \neq k} C_{kj}^{s,a} \bar{\psi}_j^{s,a}(t) \psi_k^{s,a}(t) \tag{53}$$

$$E_{n3}^{s,a}(t) = \sum_k \frac{\hbar^2}{2m}\left(\frac{k\pi}{2s(t)}\right)^2 \bar{\psi}_k^{s,a}(t) \psi_k^{s,a}(t) + \mathrm{i}\hbar \frac{\dot{s}(t)}{s(t)} \sum_k \sum_{j \neq k} C_{kj}^{s,a} \psi_j^{s,a}(t) \bar{\psi}_k^{s,a}(t). \tag{54}$$

The derivations of equations (52) and (54) by means of the orthogonality relations (12) are obvious, whereas equation (53) has been obtained from

$$E_{n2}^{s,a}(t) = \pm \mathrm{i}\hbar \frac{\dot{s}(t)}{s(t)} \sum_k \sum_j J_{jk}^{s,a} \bar{\psi}_j^{s,a}(t) \psi_k^{s,a}(t) \qquad j \gtreqless k \tag{55}$$

where

$$J_{jk}^{s,a} \equiv \frac{k}{s(t)} \int_{-s(t)}^{+s(t)} \frac{\pi}{2} \frac{x}{s(t)} \begin{matrix}\cos \\ \sin\end{matrix}\left(j \frac{\pi}{2} \frac{x}{s(t)}\right) \begin{matrix}\sin \\ \cos\end{matrix}\left(k \frac{\pi}{2} \frac{x}{s(t)}\right) \mathrm{d}x = \pm C_{kj}^{s,a} \tag{56}$$

by equation (19). Summation of equations (52)–(54) gives for the expectation value of the particle energy

$$E_n^{s,a}(t)=\sum_k \frac{\hbar^2}{2m}\left(k\frac{\pi}{2s(t)}\right)^2 \bar{\psi}_k^{s,a}(t)\psi_k^{s,a}(t)$$

$$+i\hbar\frac{\dot{s}(t)}{s(t)}\sum_k\sum_{j\neq k} C_{kj}^{s,a}(\bar{\psi}_j^{s,a}(t)\psi_k^{s,a}(t)+\psi_j^{s,a}(t)\bar{\psi}_k^{s,a}(t)). \qquad (57)$$

The complex term in equation (57) vanishes since the matrix is skew-symmetric, $C_{kj}^{s,a}=-C_{jk}^{s,a}$. Thus, we find for the average energy of the particle in the contracting or expanding box the simple but fundamental result

$$E_n^{s,a}(t)=\frac{\hbar^2}{2m}\left(\frac{n\pi}{2s(t)}\right)^2\sum_k\left(\frac{k}{n}\right)^2\bar{\Psi}_k^{s,a}(t)\Psi_k^{s,a}(t) \qquad k=\begin{cases}1,3,5,\ldots\\2,4,6,\ldots\end{cases} \qquad (58)$$

The Fourier series (58) represents a continuous function of time for $0\leq t\leq\hat{t}$. Accordingly, the energy eigenvalues $E_n^{s,a}(t)$ of the particle form a continuous spectrum in t space for any initial s,a state n.

$E_n^{s,a}(t)$ reduces to the initial energy (47) for $t\to 0$ since $\Psi_k^{s,a}(\tau=\ln(s(t)/a))\to\delta_{kn}$ for $s(t)\to a$ in equation (58). It is seen that

$$\begin{aligned}&E_n^{s,a}(t)<E_n^{s,a}(0) &&\text{for } s(t)>a\\ &E_n^{s,a}(t)>E_n^{s,a}(0) &&\text{for } s(t)<a.\end{aligned} \qquad (59)$$

Accordingly, the particle energy $E_n^{s,a}(t)$ (i) increases or (ii) decreases with time depending on whether the box is (i) compressed or (ii) expanded. This transient behaviour is explained by the uncertainty principle according to which the particle expectation energy $E_n^{s,a}(t)=\langle p_n^{s,a}(t)^2/2m\rangle$ must (i) increase and (ii) decrease with time as the particle position uncertainty $\Delta x_n^{s,a}(t)\sim s(t)$ is (i) decreased and (ii) increased by compression and expansion of the box, respectively.

5. Uncertainty relation

According to the general uncertainty principle derived by means of the Schwartz inequality the variances Δp_i and Δq_i of the non-commuting i components of the conjugate dynamical variables $\boldsymbol{p}$ and $\boldsymbol{q}$ are interrelated by the inequality $\Delta p_i\,\Delta q_i\geq\hbar/2$, that is, for any microscopic system $\Delta p_i\,\Delta q_i=\varepsilon_i\hbar/2$ where $\varepsilon_i\geq 1$ is a characteristic constant for every stationary system depending on its quantum numbers. For a proper transient system, such as a particle contained between moving walls, one expects the state function to be time dependent, $\varepsilon_i=\varepsilon_i(t)$.

The variances of the position and momentum of the particle between moving walls at $x=\pm s(t)$ are given by $(\Delta x^{s,a})^2=\langle(x^{s,a}-\langle x^{s,a}\rangle)^2\rangle=\langle(x^{s,a})^2\rangle$ and $(\Delta p^{s,a})^2=\langle(p^{s,a}-\langle p^{s,a}\rangle)^2\rangle=\langle(p^{s,a})^2\rangle$, since $\langle x^{s,a}\rangle=0$ and $\langle p^{s,a}\rangle=0$ for reasons of symmetry (see figure 1). Accordingly (initial-state subscript n omitted)

$$(\Delta p^{s,a})^2=-\hbar^2\int_{-s(t)}^{+s(t)}\bar{\psi}^{s,a}(x,t)\frac{\partial^2}{\partial x^2}\psi^{s,a}(x,t)\,dx \qquad (60)$$

$$(\Delta x^{s,a})^2=\int_{-s(t)}^{+s(t)}\bar{\psi}^{s,a}(x,t)x^2\psi^{s,a}(x,t)\,dx. \qquad (61)$$

Since their Fourier series can be differentiated term by term for the boundary conditions (3), the symmetric (s) and antisymmetric (a) wavefunctions (43) yield

$$(\Delta p^{s,a})^2 = (\hbar\pi/2s(t))^2 \sum_k k^2 \bar{\psi}_k^{s,a}(t)\psi_k^{s,a}(t) \tag{62}$$

$$(\Delta x^{s,a})^2 = \tfrac{1}{3}s(t)^2 \sum_j \sum_k \Omega_{jk}^{s,a} \bar{\psi}_j^{s,a}(t)\psi_k^{s,a}(t) \tag{63}$$

where

$$\Omega_{jk}^{s,a} = 3\left(\frac{2}{\pi}\right)^3 \int_{-\pi/2}^{+\pi/2} \xi^2 \,{}^{\cos}_{\sin}(j\xi)\,{}^{\cos}_{\sin}(k\xi)\,\mathrm{d}\xi = \Omega_{kj}^{s,a}, \tag{64}$$

that is,

$$\Omega_{jk}^{s,a} = 1 \pm 6\cos k\pi/\pi^2 k^2 \qquad j = k \tag{65}$$

$$\Omega_{jk}^{s,a} = 3\pi\left(\frac{2}{\pi}\right)^3 \left(\frac{\cos(j-k)\pi/2}{(j-k)^2} \pm \frac{\cos(j+k)\pi/2}{(j+k)^2}\right) \qquad j \neq k. \tag{66}$$

Combining equations (62) and (63) yields the time-dependent uncertainty relation for a particle in the contracting or expanding box:

$$\Delta p^{s,a}(t)\Delta x^{s,a}(t) = \tfrac{1}{2}\hbar\varepsilon^{s,a}(t) \tag{67}$$

where

$$\varepsilon^{s,a}(t) = \frac{\pi}{3^{1/2}}\Bigg(\sum_k k^2 \bar{\Psi}_k^{s,a}(t)\Psi_k^{s,a}(t) \sum_j \sum_k \Omega_{jk}^{s,a} \bar{\Psi}_j^{s,a}(t)\Psi_k^{s,a}(t)$$
$$\times \exp\left[-\frac{i\hbar}{2m}\left(\frac{\pi}{2}\right)^2 (k^2 - j^2)\int_0^t \frac{\mathrm{d}t'}{s(t')^2}\right]\Bigg)^{1/2}. \tag{68}$$

The result (68) shows that the uncertainty product (67) is real and time dependent for a particle contained between moving walls at $x = \pm s(t)$. In the limit $t \to 0$, equation (68) reduces to the state function of a particle between fixed walls

$$\lim_{t\to 0} \varepsilon^{s,a}(t) = \frac{\pi}{3^{1/2}} n(1 \pm 6\cos n\pi/\pi^2 n^2)^{1/2} \qquad n = \begin{cases} 1, 3, 5, \ldots \\ 2, 4, 6, \ldots \end{cases} \tag{69}$$

since $\Psi_j^{s,a}(t) \to \delta_{jn}$ and $\Psi_k^{s,a}(t) \to \delta_{kn}$ for $s(t) \to a$ by equation (38). As to order of magnitude, equations (62) and (63) indicate that $\Delta p^{s,a}(t) \sim \Delta p^{s,a}(0)a/s(t)$ and $\Delta x^{s,a}(t) \sim s(t)$. For this reason, the uncertainty product $(\hbar/2)\varepsilon^{s,a}(t)$ (i) decreases with t in case of compression and (ii) increases with t in case of expansion of the box (equation (68)), but only slightly since $\tau = \ln(s(t)/a)$. Comparison of equations (58) and (62) reveals that the particle energy $E^{s,a}(t)$ equals at all times the energy $\Delta p^{s,a}(t)^2/2m$ of the momentum uncertainty for any initial state n,

$$\Delta p^{s,a}(t)^2/2m = E^{s,a}(t) \qquad 0 \leq t < \hat{t}. \tag{70}$$

It follows that, on average, the walls perform (i) positive or (ii) negative work on the particle if the box is (i) compressed or (ii) expanded.

The results presented can be understood within the frame of the statistical interpretation of quantum mechanics (Schiff 1955).

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