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Semiclassical path representation of the Green function in one-dimensional multiple-well potentials

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Abstract. Using semiclassical approximations and graph-theoretical concepts, a path representation of the energy-dependent Green function in a one-dimensional multiple-well potential is derived. Applying uniform semiclassical methods, this representation is valid for energies close to the barrier maxima, where tunnelling and above-barrier reflection are of importance. Semiclassical quantization is discussed and a closed path representation of the density of states is derived. Applications to wavepacket dynamics and to the quantization of disordered systems are presented.

1. Introduction

Semiclassical methods in quantum mechanics make it possible to express quantum mechanical amplitudes in terms of the quantities characterizing the corresponding classical mechanics [1, 2]. This provides an intuitive insight into the physics under consideration and very often the semiclassical approach is a valuable tool from a purely computational point of view, when other approximation methods fail. In this paper a one-dimensional multiple-well potential is investigated. New experimental developments in solid state physics (multilayer structures, superlattices) have renewed the interest in such low-dimensional systems [3, 4].

The main result of this paper is a semiclassical *path representation* of the energy-dependent Green function $G_E(x, x')$. For its derivation use is made of elementary graph theory and of the transfer-matrix method of one-dimensional semiclassical mechanics. Therefore it is assumed that the potential $V(x)$ may be divided into N classically allowed wells where the JWKB approximation holds. Using *uniform* semiclassical transfer-matrices, the resulting representation of G_E holds when E passes across any of the maxima of $V(x)$. In this respect, the present results generalize corresponding results based on the primitive semiclassical approximation, which break down for energies close to a barrier maximum. It should be mentioned, however, that these uniform results are not valid for energies close to the minima of $V(x)$, since the matching between two barriers is performed with the primitive JWKB approximation inside the well. Based on this representation of $G_E(x, x')$, the semiclassical quantization is developed in two ways. First, following the work of Gutzwiller [5], Balian and Bloch [6], Miller [7] and Berry [1, 8], a closed-path representation of the density of states is derived. Then attention is turned to the derivation of a semiclassical quantization condition in terms of the contributions of semiclassical cycles describing the possible motions of the particle.

Two applications showing the variety of phenomena which find a description within these concepts are presented. First an example from time-dependent quantum mechanics is chosen, namely, the evolution of a wavepacket in one-dimensional multiple-well potentials. The *wavepacket autocorrelation function* is determined in a semiclassical approximation. This is a convenient quantity in investigations of time-dependent phenomena [9].

As a second application, the density of states of a disordered system is determined. Such investigations are carried out to describe the electronic properties of disordered solids (liquid metals, amorphous substances, alloys) [10–12]. It turns out that disorder leads to an exponential suppression of long cycles. Thus, taking into account only the shortest cycles, the main features of the density of states are already reproduced.

It is to be emphasized that the results of this paper are based only on the existence of transfer-matrices to determine the solution of Schrödinger's equation with given boundary conditions inside a certain well. In this respect, the restriction to a *semiclassical* path representation can be abolished whenever exact transfer-matrices are available (e.g. in Kronig–Penney-type potentials). For such model potentials the results are rigorous.

2. Path representation of the Green function

In this section a semiclassical expression for the time-independent Green function $G_E(x, x')$ solving the inhomogenous Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + [V(x) - E]\right) G_E(x, x') = \delta(x - x') \quad (1)$$

of a one-dimensional multiple-well potential $V(x)$ is derived. This representation is *uniformly* valid if the energy passes across a barrier maximum. This goes beyond an asymptotic first-order \hbar -expansion, which is not valid for energies close to the barrier maxima. As already mentioned in the first section, the results are not valid for energies lower than the highest of the minima of $V(x)$.

The starting point is the transfer-matrix method of semiclassical mechanics [1, 2]. These so-called connection formulae relate local semiclassical solutions on both sides of a barrier. Then it is shown how this result can be rewritten as a *path representation*, using basic concepts of graph theory [13, 14]. Based on a first-order \hbar (classical) path representation of G_E Gutzwiller [5] derived a closed-path representation for the density of states (see section 3) for multidimensional systems which, however, does not take into account quantum-mechanical tunnelling. Using complex paths, Balian and Bloch [6] developed a so-called *multiple-scattering* expansion to obtain arbitrary higher-order \hbar -corrections to G_E in multidimensional systems. In this respect, the use of uniform semiclassical transfer-matrices in the energy region around the maxima may be viewed as a partial summation of Balian and Bloch's expansion for G_E .

The potential $V(x)$ considered here consists of N wells separated by $N - 1$ barriers (figure 1). For given energy E , the left (right) classical turning point of the n th well is denoted by $x_{<}^n$ ($x_{>}^n$), respectively. For energies E above the n th barrier maximum $V_{\max}^n = V(x_{\max}^n)$, the two turning points become complex. However, the (real) above-barrier reflection point x_r^n as defined in appendix A allows one to fix

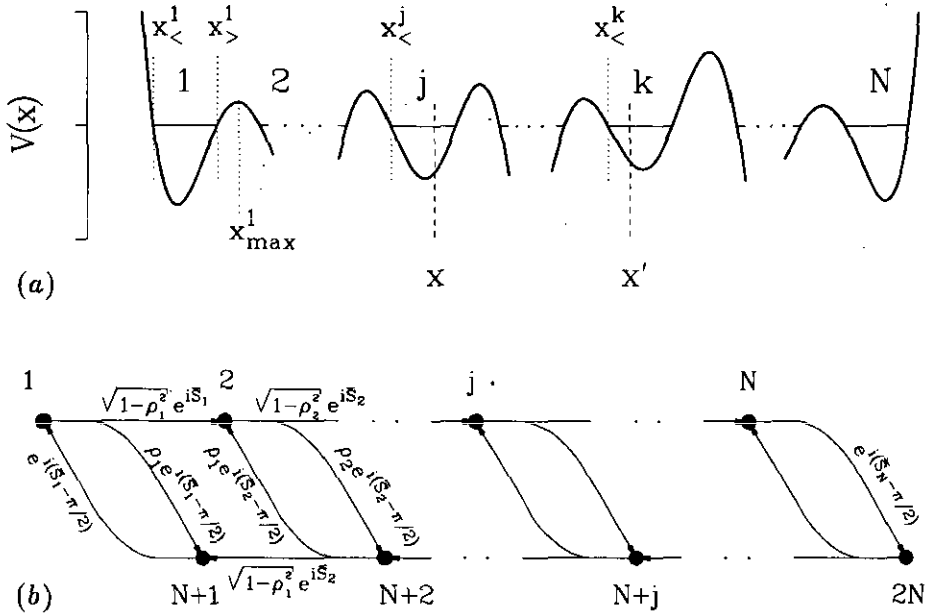


Figure 1. (a) Multiple-well potential; (b) corresponding weighted graph according to the adjacency matrix \mathcal{A} . Some weights $w(i, j)$ are indicated.

$x_{>}^n = x_{<}^{n+1} = x_r^n$. If the n th barrier is symmetric, one has $x_r^n \equiv x_{\max}^n$ for all energies $E > V_{\max}^n$.

The semiclassical solution $\psi(x)$ of Schrödinger's equation for positions x well inside the j th well ($x_{<}^j \ll x \ll x_{>}^j$) reads [1, 2]

$$\psi(x) = \frac{1}{\sqrt{k(x)}} (Ae^{+iS(x_{<}^j, x)} + Be^{-iS(x_{<}^j, x)}).$$

As usual, $k(x) = \sqrt{2\mu[E - V(x)]}/\hbar$ is the wavenumber and $S(x_1, x_2) = \int_{x_1}^{x_2} dx k(x)$ is the classical action from x_1 to x_2 in units of \hbar . The coefficients A, B have to be determined by appropriate boundary conditions. As an example, in the first well ($j = 1$), to ensure exponential decay for $x \rightarrow -\infty$, one has $(A_1, B_1) = C(e^{-i\pi/4}, e^{i\pi/4})$ (C is a suitably chosen normalization factor). Therefore

$$\psi(x) = \frac{2C}{\sqrt{k(x)}} \cos[S(x_{<}^1, x) - \pi/4] \quad \text{for} \quad x_{<}^1 \ll x \ll x_{>}^1$$

the well known JWKB solution.

Due to the linearity of the Schrödinger equation, the corresponding coefficients (A_j, B_j) for $x_{<}^j \ll x \ll x_{>}^j$ are obtained from (A_1, B_1) with the help of a (2×2) transfer-matrix [1, 2], i.e.

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \mathbf{K}(j_{<} \leftarrow 1_{<}) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}.$$

The matrix $\mathbf{K}(j_{<} \leftarrow 1_{<})$ from $x_{<}^1$ to $x_{<}^j$ is a composition of the elementary transfers through each well (matrices \mathbf{L}) and through each barrier (matrices \mathbf{M}), i.e.

$$\mathbf{K}(j_{<} \leftarrow 1_{<}) = \mathbf{M}(j_{<} \leftarrow (j-1)_{>}) \cdots \mathbf{M}(2_{<} \leftarrow 1_{>}) \mathbf{L}(1_{>} \leftarrow 1_{<}) \quad (2)$$

with

$$\mathbf{L}(n_{>} \leftarrow n_{<}) = \begin{pmatrix} e^{iS_n} & 0 \\ 0 & e^{-iS_n} \end{pmatrix}$$

and

$$\mathbf{M}((n+1)_{<} \leftarrow n_{>}) = (1 - \rho_n^2)^{-1/2} \begin{pmatrix} e^{-i\phi_n} & -i\rho_n \\ i\rho_n & e^{i\phi_n} \end{pmatrix}.$$

Here, $S_n = S(x_{<}^n, x_{>}^n)$ is the classical action through the n th well, ρ_n is the reflection amplitude and ϕ_n is the scattering phase shift of the n th barrier. The semiclassical expressions for these quantities are obtained by mapping the barrier onto an inverse parabola [15, 1] and are listed in appendix A.

The energy-dependent Green function $G_E(x, x')$ of equation (1) is determined with the help of two solutions $\psi_{<}(x), \psi_{>}(x)$ of the Schrödinger equation fulfilling the boundary conditions $\psi_{<}(x) \xrightarrow{x \rightarrow -\infty} 0$ and $\psi_{>}(x) \xrightarrow{x \rightarrow +\infty} 0$. Use is made of the representation [16]

$$G_E(x, x') = \frac{2\mu}{\hbar^2} \frac{\psi_{<}(x_{\min})\psi_{>}(x_{\max})}{\mathcal{W}(\psi_{<}, \psi_{>})} \quad (3)$$

with $x_{\min} := \min(x, x')$, $x_{\max} := \max(x, x')$ and the Wronskian

$$\mathcal{W}(\psi_{<}, \psi_{>}) = \psi_{<}\psi'_{>} - \psi'_{<}\psi_{>}.$$

Assuming that $x < x'$, and that x is situated in the well j ($x_{<}^j \ll x \ll x_{>}^j$) and x' in the well k ($j \leq k$), the quantities in equation (3) can be determined semiclassically with the given connection formulae. For this purpose, the transfer-matrix $\mathbf{K}(j_{<} \leftarrow 1_{<})$ (equation (2)) has to be determined and corresponding expressions for the matrices $\mathbf{K}(k_{>} \leftarrow N_{>})$ and $\mathbf{K}(N_{>} \leftarrow 1_{<})$. Letting

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \mathbf{K}(j_{<} \leftarrow 1_{<}) \begin{pmatrix} e^{-i\pi/4} \\ e^{i\pi/4} \end{pmatrix}$$

and

$$\begin{pmatrix} \kappa_1 \\ \kappa_2 \end{pmatrix} = \mathbf{K}(k_{>} \leftarrow N_{>}) \begin{pmatrix} e^{i\pi/4} \\ e^{-i\pi/4} \end{pmatrix}$$

one obtains in semiclassical approximation

$$\psi_{<}(x) = \frac{C_{<}}{\sqrt{k(x)}} \{ \lambda_1 e^{+iS(x_{<}^j, x)} + \lambda_2 e^{-iS(x_{<}^j, x)} \} \quad \text{for } x_{<}^j \ll x \ll x_{>}^j$$

$$\psi_{>}(x') = \frac{C_{>}}{\sqrt{k(x')}} \{ \kappa_1 e^{+iS(x_{>}^k, x')} + \kappa_2 e^{-iS(x_{>}^k, x')} \} \quad \text{for } x_{<}^k \ll x' \ll x_{>}^k$$

and

$$W(\psi_<, \psi_>) = 2C_<C_> \text{Tr} \left[\mathbf{K}(N_> \leftarrow 1_<) \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \right] \tag{4}$$

with $\text{Tr}\{\dots\}$ denoting the trace of the 2×2 matrix. Then equation (3) reads

$$G_E(x, x') = \frac{\mu}{\hbar^2} (k(x)k(x'))^{-1/2} \times \sum_{m,n=1}^2 \{ \lambda_m \kappa_n e^{i(\pm S(x_<^j, x) \pm S(x_>^k, x'))} \} / \text{Tr} \left[\mathbf{K}(N_> \leftarrow 1_<) \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \right]. \tag{5}$$

As has been worked out by Miller [7] for the case $N = 2$, it is possible to expand the quotient $1/\text{Tr}\{\dots\}$ in (5) in (multiple) geometric series. Assuming that $V_{\min}^{(1,2)} \ll E \ll V_{\max}$ and therefore taking into account only contributions of order $(\sqrt{1 - \rho^2})^2$ (for $j = k$), each summand of the series may be assigned to a path that passes back and forth in the first well, then tunnels and passes back and forth in the second well before it tunnels back.

Using the basic concepts of graph theory, however, (5) can be converted into a semiclassical path representation of the Green function for arbitrary N and all energies $E \gg V_{\min}^i$ ($i = 1, \dots, N$) by expanding G_E in a single (matrix) geometrical series. The main step is to combine all entries of the 2×2 transfer-matrices involved in equation (5) in a single $(2N \times 2N)$ matrix

$$\mathcal{A} = \begin{pmatrix} \mathcal{A}_1 & \mathcal{A}_2 \\ \mathcal{A}_3 & \mathcal{A}_4 \end{pmatrix}. \tag{6}$$

The four $(N \times N)$ matrices $\mathcal{A}_1, \dots, \mathcal{A}_4$ are defined as

$$\begin{aligned} (\mathcal{A}_1)_{ij} &= \delta_{ij-1} \sqrt{1 - \rho_i^2} e^{i\bar{S}_i}, \\ (\mathcal{A}_2)_{ij} &= \delta_{ij} \rho_i e^{i(\bar{S}_i - \pi/2)} \\ (\mathcal{A}_3)_{ij} &= \delta_{ij} \rho_{i-1} e^{i(\bar{S}_i - \pi/2)} \\ (\mathcal{A}_4)_{ij} &= \delta_{ij+1} \sqrt{1 - \rho_{i-1}^2} e^{i\bar{S}_i}. \end{aligned} \tag{7}$$

To simplify the notation, *modified actions*

$$\bar{S}_n = S_n - \frac{1}{2} \{ \phi_{n-1} + \phi_n \} \tag{8}$$

are defined, such that \bar{S}_n approaches the classical action S_n for energies far above or far below the barrier maxima, since the phase shifts ϕ_{n-1}, ϕ_n go to zero in these limits (equation (A3)). The phase shifts imply that the time $\bar{T}_n = d\bar{S}_n/dE$ remains finite for energies close to a barrier maximum. This is in contrast to the *classical* orbiting time $T_n = dS_n/dE$ from $x_n^<$ to $x_n^>$, which tends to infinity for energies equal to the barrier maxima $E = V_{\max}^{n-1}$ or $E = V_{\max}^n$.

With this $(2N \times 2N)$ matrix \mathcal{A} , one obtains from equation (5) for the Green function for values $x^j_{<} \ll x \ll x^j_{>}$ and $x^k_{<} \ll x' \ll x^k_{>}$

$$\begin{aligned}
 G_E(x, x') = & \frac{i\mu}{\hbar^2} [k(x)k(x')]^{-1/2} \{ [(\mathbb{1} - \mathcal{A})^{-1}]_{j,k} e^{-i\bar{S}(x^j_{<}, x) + i\bar{S}(x^k_{>}, x')} \\
 & + [(\mathbb{1} - \mathcal{A})^{-1}]_{j, N+k} e^{-i\bar{S}(x^j_{<}, x) + i\bar{S}(x', x^k_{>})} \\
 & + [(\mathbb{1} - \mathcal{A})^{-1}]_{N+j, k} e^{-i\bar{S}(x, x^j_{>}) + i\bar{S}(x^k_{<}, x')} \\
 & + [(\mathbb{1} - \mathcal{A})^{-1}]_{N+j, N+k} e^{-i\bar{S}(x, x^j_{>}) + i\bar{S}(x', x^k_{>})} \} . \tag{9}
 \end{aligned}$$

Note that each of the four summands in (9) corresponds to one of the summands in equation (5).

The equivalence of equations (5) and (9) can be shown with the derivation of equivalent (two-dimensional) recurrence relations $N \rightarrow (N + 1)$ for both equations. In equation (5), the step $N \rightarrow (N + 1)$ is performed by multiplying the transfer-matrices with an additional (2×2) matrix. By contrast, in (9), it is performed by enlarging the $(2N \times 2N)$ matrix \mathcal{A} by two new rows and columns.

The matrix \mathcal{A} may be interpreted as the *weighted adjacency matrix* of a graph [14, 15]. To become familiar with this terminology, basic definitions and concepts of graph theory are listed in appendix B. Here, use is made of the identity (B3),

$$[(\mathbb{1} - \mathcal{A})^{-1}]_{jk} = \delta_{jk} + \sum_{\gamma_{j \rightarrow k}} w(\gamma_{j \rightarrow k}) \tag{10}$$

to express the inverse $(\mathbb{1} - \mathcal{A})^{-1}$ entering (9) as a sum of weights $w(\gamma)$ over certain paths γ of the corresponding graph. In our case, the matrix \mathcal{A} represents the graph shown in the bottom of figure 1. A *path* $\gamma_{i \rightarrow j}$ from vertex i to j is a sequence of connected vertices of the graph. Its *weight* $w(\gamma_{i \rightarrow j})$ is the product of the weights of all edges it consists of. These elementary weights of the edges are determined by the adjacency matrix, i.e. $w(i, j) = A_{ij}$. Notice that the series on the right-hand side of (10) is convergent for energies with $\text{Im}(E) > 0$ since the actions \bar{S}_i in (7) have a positive imaginary part too. The graph in figure 1 can be interpreted as a phase-space portrait of the possible (tunnelling and reflecting) paths along which a semiclassical particle evolves, each edge weighted with appropriate phases and amplitudes. The upper edges $(1, 2), \dots, ((N - 1), N)$ are edges of positive momentum. Along the lower edges, however, the motion has negative momentum.

Now turning back to (9) and using (10) in each of the four summands one sees that (9) provides a *path representation* of G_E . The first summand in (9) is the contribution of all paths emerging from x with positive momentum (vertex j) and arriving at x' with positive momentum (vertex k). The additional factor $e^{-i\bar{S}(x^j_{<}, x) + i\bar{S}(x^k_{>}, x')}$ fixes the actual starting and end point (x, x') instead of $(x^j_{<}, x^k_{>})$. Accordingly, the second summand is the contribution of all paths emerging from x with positive momentum (vertex j) and arriving at x' with negative momentum (vertex $N + k$). The third (fourth) summand is the contribution of all paths emerging from x with negative momentum (vertex $N + j$) and arriving at x' with positive (negative) momentum (vertex $k, (N + k)$), respectively.

Thus for energies with $\text{Im}(E) > 0$, equation (9) can be written formally as

$$G_E(x, x') = \frac{i\mu}{\hbar^2} [k(x)k(x')]^{-1/2} \sum_{\gamma_{x \rightarrow x'}} w(\gamma_{x \rightarrow x'}) . \tag{11}$$

Equation (11) is the desired path representation of the Green function in a multiple-well potential. Here, the summation is extended over all paths $\gamma_{x \rightarrow x'}$ which lead from x to x' in the sense of the graph in figure 1, with corresponding weights $w(\gamma_{x \rightarrow x'})$, given by the product of all coefficients A_{ij} along the path $\gamma_{x \rightarrow x'}$. In general, the weight of a path will be written as

$$w(\gamma) = \Lambda_\gamma e^{i(\bar{S}_\gamma - m_\gamma \pi/2)} \quad (12)$$

with the product of the reflection and transmission amplitudes

$$\Lambda_\gamma = \prod_{n=1}^{N-1} \rho_n^{r_n} (\sqrt{1 - \rho_n^2})^{t_n}$$

the indices r_n (t_n) denoting the number of reflections (transmissions) at the n th barrier. The sum of all modified actions of the path is \bar{S}_γ , and m_γ denotes the number of reflections.

The behaviour of these results as E passes across a maximum of $V(x)$ may be understood clearly by looking at the graph in figure 1. For energies E well above all maxima of $V(x)$, all reflection amplitudes ρ_i tend to zero. This implies that the weights of the inner edges of the graph tend to zero which means that these edges may be removed. Thus, the resulting graph represents a single large well. On the other hand, if E is well below all maxima, the graph splits into N disconnected pieces, since the weights of the horizontal edges tend to zero. The resulting graph represents N independent wells. More of these limiting behaviours will be discussed in section 4.

It is worth noting that probability conservation leads to a *node rule* for each vertex i ($i = 1, \dots, 2N$), i.e.

$$\sum_{j=1}^{2N} (|A_{ji}|^2 - |A_{ij}|^2) = 1 - 1 = 0$$

in analogy to Kirchhoff's rule $\sum I_j = 0$ for each node in an electrical circuit. This results from the unitarity of the adjacency matrix \mathcal{A}

$$\mathcal{A}^\dagger \mathcal{A} = \mathbb{1}.$$

The representation (11) turns out to be useful for investigations in wavepacket dynamics (section 4), but also serves as starting point for a concise formulation of the semiclassical quantization of these potentials, as will be shown in the following sections.

3. Density of states

In this section the density of states $d(E)$ of a multiple-well system is considered by making use of the corresponding graph and its associated adjacency matrix \mathcal{A} . In general, taking the trace of the Green function leads directly to the density of states. In a first-order \hbar -approximation it is therefore possible to express $d(E)$ in terms

of closed classical paths of the (multidimensional) system. This has been worked out by Gutzwiller and others [5,8]. Balian and Bloch [6] derived analogous (exact) results including complex closed paths. Miller and others [7,17,18] applied closed-path quantization to systems including tunnelling. In the present work, the density of states will be expressed in terms of closed paths of the graph (figure 1), which will be applied to the quantization of disordered systems in section 5. To determine the density of states

$$d(E) = \sum_{n=1}^{\infty} \delta(E - E_n)$$

the eigenenergies of the system being denoted by E_n , use is made of

$$d(E) = -\frac{1}{\pi} \text{Im}[\text{Tr}(G_E)]. \tag{13}$$

The integration $\text{Tr}(G_E) = \int dx G_E(x, x)$ can be carried out using (3) and the Schrödinger equation for $\psi_<, \psi_>$, leading to $\text{Tr}(G_E) = d/dE \ln [\mathcal{W}(\psi_<, \psi_>)]$. In the semiclassical approximation the Wronskian is given by (4). Similarly to the equivalence of (5) and (9), the Wronskian of (4) may be expressed using the $(2N \times 2N)$ matrix \mathcal{A} . This leads to

$$\mathcal{W}(\psi_<, \psi_>) = 2C_< C_> \left(\prod_{i=1}^{N-1} (1 - \rho_i^2)^{-1/2} e^{-i\bar{S}/2} \det(\mathbb{1} - \mathcal{A}) \right) \tag{14}$$

with $\bar{S} = 2 \sum_{i=1}^N \bar{S}_i$. For energies well above and well below all barrier maxima the scattering phase shifts vanish and one has $\bar{S} = 2 \sum S_i$, the classical phase space volume of the system in units of \hbar . One finds

$$\text{Tr}(G_E) = \frac{d}{dE} \ln \left(\prod_{i=1}^{N-1} (1 - \rho_i^2)^{-1/2} e^{-i\bar{S}/2} \det(\mathbb{1} - \mathcal{A}) \right)$$

and from (13)

$$d(E) = \bar{d}(E) - \frac{1}{\pi} \text{Im} \left(\frac{d}{dE} \ln[\det(\mathbb{1} - \mathcal{A})] \right). \tag{15}$$

Here,

$$\bar{d}(E) = \frac{1}{2\pi} \frac{d\bar{S}}{dE} = \frac{\bar{T}}{2\pi\hbar}$$

denotes the average density of states. The oscillating part of the density of states

$$d_{\text{osc}}(E) = -\frac{1}{\pi} \text{Im} \left(\frac{d}{dE} \ln[\det(\mathbb{1} - \mathcal{A})] \right) \tag{16}$$

can again be treated applying graph-theoretical concepts. Using $\ln[\det(B)] = \text{Tr}(\ln(B))$ for a matrix B one obtains

$$\ln[\det(\mathbb{1} - \mathcal{A})] = - \sum_{m=1}^{\infty} \frac{1}{m} \text{Tr}[(\mathcal{A})^m] = - \sum_{m=1}^{\infty} \frac{1}{m} \sum_{\substack{\gamma \text{ closed} \\ |\gamma|=m}} w(\gamma) \tag{17}$$

where use is made of the fact that $(\mathcal{A}^m)_{kk}$ is equal to the sum of the weights of all closed paths from vertex k back to k of length $|\gamma| = m$ (equation (B2)). Now the quantity of central interest in (16) is expressed in terms of the closed paths γ of the corresponding graph and their weights $w(\gamma)$.

The weight of the closed path $\gamma_{k_1 \rightarrow k_1} = (k_1 k_2 \dots k_m k_1)$ from k_1 back to k_1 is equal to the weight of the closed paths $\gamma_{k_2 \rightarrow k_2} = (k_2 k_3 \dots k_m k_1 k_2), \dots, \gamma_{k_m \rightarrow k_m} = (k_m k_1 \dots k_m)$ which are obtained from $\gamma_{k_1 \rightarrow k_1}$ by shifting the beginning vertex. All these closed paths represent what will be called the same *cycle* $[\gamma]$ of the graph. In general, a path γ ($|\gamma| = m$) is a j -fold repetition of a shortest, so-called *primitive* closed path γ^P , ($|\gamma^P| = m/j$). Therefore, the number $N_{[\gamma]}$ of different closed paths representing the same cycle $[\gamma]$ of length m is $N_{[\gamma]} = |\gamma^P| = m/j$. Expressing the sum over all closed paths in (17) as a sum over cycles, one finds

$$\ln[\det(\mathbb{1} - \mathcal{A})] = - \sum_{[\gamma]} \frac{1}{j} w(\gamma) = \sum_{[\gamma^P]} \ln[1 - w(\gamma^P)]. \quad (18)$$

For the second equation, the summation over all cycles $[\gamma]$ is replaced by a summation over all primitive cycles $[\gamma^P]$ and their j -fold repetitions. Thus, from (16), (18) and (12), for energies with $\text{Im}(E) > 0$ the oscillating part of the density of states is finally given by

$$d_{\text{osc}}(E) = \frac{1}{\pi \hbar} \text{Re} \left[\sum_{[\gamma^P]} \left(\overline{T}_\gamma - i \hbar \frac{\Lambda'_\gamma}{\Lambda_\gamma} \right) \sum_{m=1}^{\infty} (\Lambda_\gamma)^m e^{im(\overline{S}_\gamma - m\gamma\pi/2)} \right]. \quad (19)$$

Again, $\overline{T}_\gamma = \hbar(d\overline{S}_\gamma/dE)$ is the modified orbiting time and $\Lambda'_\gamma = (d\Lambda_\gamma/dE)$. The formal structure of (19) is equivalent to those obtained in a first-order \hbar -expansion in (higher-dimensional) semiclassical mechanics [5, 8, 18], the *classical* orbiting time T_γ being replaced by the *complex*, modified time $(\overline{T}_\gamma - i\hbar\Lambda'_\gamma/\Lambda_\gamma)$. This results from the *uniform* semiclassical approximation, also valid for energies close to the barrier maxima.

In general, (19) is not suitable for the calculation of eigenenergies of a given multiple-well potential since, to arrive at a sufficient energy resolution, high frequencies (i.e. long cycles) have to be taken into account. In some cases, however, when high frequencies are suppressed (e.g. because of a finite energy resolution of the detector or, equivalently, giving E a positive imaginary part) (19) will be a *convergent* series and a few short cycles will already give an accurate result. Another example is given in section 5, by quantizing a disordered multiple-well potential, where disorder leads to an exponential suppression of long cycles.

4. Semiclassical quantization

To determine the eigenenergies of a given N -minima potential it is more convenient to find a semiclassical *quantization condition*, i.e. a function $f_N(E)$ having the property $f_N(E) = 0$ if E is an eigenenergy of the system. In one-dimensional systems the desired quantization condition reads $\mathcal{W}(\psi_<, \psi_>)(E) = 0$. Equation (14) shows that in semiclassical approximation, this is equivalent to the condition

$$f_N(E) = e^{-i\overline{S}/2} \det(\mathbb{1} - \mathcal{A}) = 0. \quad (20)$$

The factor $e^{-i\bar{S}/2}$ ensures $f_N(E)$ is real for real energies, which is comfortable from a computational point of view. In reference [19], Bogomolny derived a similar quantization condition for the energy levels of a bound system in a first-order \hbar -approximation for the multidimensional case. The determinant in (20) could be directly computed with suitable routines. In our case a convenient way to determine $f_N(E)$ is to use the recurrence relation

$$\begin{pmatrix} f_n \\ g_n \end{pmatrix} = e^{-i\bar{S}_n} \begin{pmatrix} \rho_{n-1} + e^{2i\bar{S}_n} & (1 - \rho_{n-1})(1 - e^{2i\bar{S}_n}) \\ \rho_{n-1} & (1 - \rho_{n-1}) \end{pmatrix} \begin{pmatrix} f_{n-1} \\ g_{n-1} \end{pmatrix} \tag{21}$$

with starting value

$$\begin{pmatrix} f_1 \\ g_1 \end{pmatrix} = \begin{pmatrix} 2 \cos(\bar{S}_1) \\ \exp\{-i\bar{S}_1\} \end{pmatrix}.$$

The function $f_{(n=N)} = f_N(E)$ is the quantization function of the N -minima potential.

However, it is desirable to link the quantity $f_N(E)$ to the cycles of the corresponding potential graph (figure 1). This is achieved from (20) by a cycle interpretation of the definition of the determinant of a matrix $B = (b_{ij})$. One has $\det(B) = \sum_{\pi} \sigma(\pi) b_{1\pi(1)} b_{2\pi(2)} \dots b_{n\pi(n)}$, π running over all permutations of the numbers $1, \dots, n$ and $\sigma(\pi)$ being its sign. A permutation π may be written in *cycle form*

$$\pi = (n_{11} \dots n_{1m_1}) \dots (n_{i1} \dots n_{im_i}) \quad (1 \leq i \leq [n/2])$$

which means that π is a composition of i cyclic permutations such as $n_{11} \rightarrow n_{12} \rightarrow \dots \rightarrow n_{1m_1} \rightarrow n_{11}$. Thus any permutation π may be assigned to a set of i (primitive) cycles $\{[\gamma_1], [\gamma_2], \dots, [\gamma_i]\}_{\pi}$ of the graph with $\gamma_1 = (n_{11} \dots n_{1m_1} n_{11})$ and corresponding identifications for $\gamma_2, \dots, \gamma_i$. Writing $\{\dots\}_{\pi}$ it is stressed that the set of cycles $[\gamma_1], [\gamma_2], \dots, [\gamma_i]$ involved has to represent a *permutation* π of the n numbers. Moreover, the contribution of this permutation to the determinant may be determined with the weights of the corresponding cycles of the graph. Letting $B = (\Pi - A)$ then, since $b_{ii} = 1, b_{ij} = -A_{ij}$ for $i \neq j$, one finds

$$\sigma(\pi) b_{1\pi(1)} b_{2\pi(2)} \dots b_{(2N)\pi(2N)} = (-1)^k w(\gamma_1) w(\gamma_2) \dots w(\gamma_i).$$

Therefore, the quantization condition (20) may finally be written as

$$\begin{aligned} f_N(E) = e^{-i\bar{S}/2} \left\{ 1 - \sum_{[\gamma]_{\pi}} w(\gamma) + \sum_{\{[\gamma_1], [\gamma_2]\}_{\pi}} w(\gamma_1) w(\gamma_2) \right. \\ \left. - \dots + (-1)^N \sum_{\{[\gamma_1], \dots, [\gamma_N]\}_{\pi}} w(\gamma_1) \dots w(\gamma_N) \right\}. \tag{22} \end{aligned}$$

Starting with the contribution '1' of the identity permutation, one has to subtract the weights of all cycles $[\gamma]$ of the graph representing a cyclic permutation, then add the product of the weights of all pairs of cycles $\{[\gamma_1], [\gamma_2]\}$ of the graph which represent a permutation, and so on. For small N , (22) is easily evaluated (figure 1) as follows.

In the case $N = 1$, the only permutation of the two numbers $\{1, 2\}$ corresponding to a cycle is $\pi = (12)$ and this gives

$$f_1(E) = e^{-iS/2}(1 - e^{i(S-\pi)}) = 2 \cos(S/2)$$

which is equivalent to the Bohr-Sommerfeld quantization condition $S\hbar = \oint p dq = 2\pi(n + 1/2)\hbar$.

In the case $N = 2$, there are three permutations of the numbers $\{1, 2, 3, 4\}$ corresponding to cycles of the graph, namely (13), (24) and (1243). Moreover, the permutation (13)(24) is also represented by the graph. The corresponding weights are read from the graph, $w(13) = \rho e^{2i(\bar{S}_1 - \pi/2)}$, $w(24) = \rho e^{2i(\bar{S}_2 - \pi/2)}$ and $w(1243) = (1 - \rho^2)e^{2i(\bar{S}_1 + \bar{S}_2 - \pi/2)}$. Therefore, the quantization function (22) reads

$$\begin{aligned} f_2(E) &= e^{-i(\bar{S}_1 + \bar{S}_2)} \{1 - w(13) - w(24) - w(1243) + w(13)w(24)\} \\ &= e^{-i(\bar{S}_1 + \bar{S}_2)} \{1 - \rho e^{2i(\bar{S}_1 - \pi/2)} - \rho e^{2i(\bar{S}_2 - \pi/2)} - (1 - \rho^2)e^{2i(\bar{S}_1 + \bar{S}_2 - \pi/2)} \\ &\quad + \rho^2 e^{2i(\bar{S}_1 + \bar{S}_2 - \pi)}\} \end{aligned}$$

or equivalently (see also [2])

$$f_2(E) = \cos(\bar{S}_1 + \bar{S}_2) + \rho \cos(\bar{S}_1 - \bar{S}_2).$$

A number of 12 permutations are represented by the graph in the case $N = 3$, namely (14), (25), (36), (1254), (2365), (123654), (14)(25), (14)(36), (14)(2365), (25)(36), (1254)(36) and (14)(25)(36).

For large N the contributions of an exponentially growing number of combinations of cycles have to be taken into account in order to express the semiclassical quantization condition (20) in terms of cycles.

In order to discuss various limiting behaviours of the quantization function $f_N(E)$, (18) may be exponentiated leading to

$$f_N(E) = e^{-i\bar{S}/2} \prod_{\{\gamma^p\}} [1 - w(\gamma^p)]. \tag{23}$$

Thus an *infinite* product representation for the quantization function in terms of *all* primitive cycles of the graph is found. First, consider energies well above all maxima. In this case, as already mentioned in the second section, all inner edges of the graph vanish since the reflection amplitudes tend to zero. The resulting graph is the graph of a single well and the N -well result reduces to the Bohr-Sommerfeld quantization condition of $N = 1$ with action $S = \sum S_i$. In the opposite limit consider energies well below all maxima. Now the transmission amplitudes tend to zero and the N -minima graph reduces to N disconnected single-minimum graphs. The product over all primitive cycles in (23) reduces to the product of N single-well quantization functions which means that $f_N(E) = f_1^{(1)}(E)f_1^{(2)}(E) \dots f_1^{(N)}(E)$. Further, consider the case of a single huge k th barrier, all other barriers being much smaller. Then for energies between the smaller maxima and V_{\max}^k the transmission amplitude $\sqrt{1 - \rho_k^2}$ tends to zero and the corresponding graph splits into two pieces, representing the graphs of a k -minima and a $(N - k)$ -minima potential. The product

over all primitive cycles in (23) splits into the two infinite products over the primitive cycles of the individual graphs. Therefore the quantization function may be written in the form $f_N(E) = f_k(E)f_{(N-k)}(E)$. Due to the uniformity of the connection formulae, A and therefore the whole graph interpolates smoothly between these limiting cases.

Notice that (23) as derived is valid only for energies with a positive imaginary part—the infinite product is not convergent for real energies. Equation (23) is equal to the finite expression (22) according to an analytical continuation procedure. This can be achieved by the mechanism of the so-called *cycle expansion* [20]. Expanding

$$\prod_{[\gamma^p]} [1 - w(\gamma^p)] = 1 - \sum_{[\gamma^p]} w(\gamma^p) + \sum_{[\gamma_1^p], [\gamma_2^p]} w(\gamma_1^p)w(\gamma_2^p) - \dots \quad (24)$$

all but a finite number of terms cancel and only the contributions of the *permutation* cycles of (22) remain. In this context, the *weighted adjacency matrix* A plays the role of the *transfer operator* [20].

5. Applications

5.1. Wavepacket autocorrelation function

As a first application of the path representation concept, wavepacket dynamics in a multiple-well potential is investigated. A convenient way to exhibit the time dependence of a wavepacket $\Psi(t)$ is to evaluate its *autocorrelation function* [9]

$$a(t) = \langle \Psi(0) | \Psi(t) \rangle. \quad (25)$$

The square of this function measures the degree to which the wavepacket at time t overlaps with the initial wavepacket at $t = 0$. In this section a semiclassical expression for $a(t)$ in a multiple-well potential is derived, based on the corresponding potential graph. It is assumed that the initial wavepacket $\Psi_0 = \Psi(t = 0)$ is localized around the leftmost turning point $x_{<}^1(\bar{E})$ of a given mean energy \bar{E} (see upper right corner of figure 2). To link the time evolution $\Psi(t) = U(t)\Psi_0$ to the path representation derived in section 1 use is made of

$$U(t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} dE e^{-i(E+i\epsilon)t/\hbar} G_{E+i\epsilon}. \quad (26)$$

Therefore, the autocorrelation function $a(t)$ is the Fourier transform of the quantity

$$\langle \Psi_0 | G_E | \Psi_0 \rangle = \int dx \int dx' \Psi_0^*(x) G_E(x, x') \Psi_0(x').$$

The function $\Psi_0(x)$ is localized around $x_{<}^1$, thus for $x, x' \approx x_{<}^1$, in (3) one has to fall back on *uniform* approximations for $\psi_{<}, \psi_{>}$. Then, instead of (9) one finds for $-\infty < x, x' \ll x_{>}^1$

$$G_E(x, x') = -2\pi i \{ \psi_{<}^{re}(x_{\min}) \psi_{<}^{ir}(x_{\max}) + \sum_{\gamma_{1-1}} w(\gamma_{1-1}) \psi_{<}^{re}(x_{\min}) \psi_{<}^{re}(x_{\max}) \}. \quad (27)$$

For the derivation of (27) again use is made of (10). The (energy-normalized) regular and irregular solutions $\psi_{<}^{\text{re}}, \psi_{<}^{\text{ir}}$ in semiclassical (uniform) approximation are given by [1, 2]

$$\begin{aligned}\psi_{<}^{\text{re}}(x) &= \sqrt{\frac{2\mu}{\hbar^2}} \left(\frac{\xi(x)}{k(x)^2} \right)^{1/4} \text{Ai}(-\xi(x)) \\ \psi_{<}^{\text{ir}}(x) &= \sqrt{\frac{2\mu}{\hbar^2}} \left(\frac{\xi(x)}{k(x)^2} \right)^{1/4} \frac{1}{2} [\text{Ai}(-\xi(x)) + i\text{Bi}(-\xi(x))]\end{aligned}$$

with $\xi(x) := [3S(x_{<}^1, x)/2]^{2/3}$. The functions $\text{Ai}(z)$, $\text{Bi}(z)$ denote the regular and irregular Airy function [21]. Inserting (26) and (27) into (25) one arrives at

$$a(t) = a_0(t) + \sum_{\gamma_{1 \rightarrow 1}} a_\gamma(t). \quad (28)$$

Here, the first term

$$a_0(t) = \int dE e^{-iEt/\hbar} \left[\int dx \int dx' \Psi_0^*(x) \psi_{<}^{\text{re}}(x_{\text{min}}) \psi_{<}^{\text{ir}}(x_{\text{max}}) \Psi_0(x') \right] \quad (29)$$

is the overlap of $\Psi(t)$ with Ψ_0 for very short times (see figure 2(a)), which means before the wavepacket $\Psi(t)$ has left the region of Ψ_0 . The second term in (28) is the sum of the contributions of all possible returns $\gamma_{1 \rightarrow 1}$ of the wavepacket to the starting region around $x_{<}^1$. According to (12) and (27), the contribution $a_\gamma(t)$ of a single path $\gamma_{1 \rightarrow 1}$ is given by

$$a_\gamma(t) = e^{-im_\gamma \pi/2} \int dE |\langle \psi_{<}^{\text{re}} | \Psi_0 \rangle|^2 \Lambda_\gamma(E) e^{-i(Et - \hbar \bar{S}_\gamma)/\hbar}. \quad (30)$$

For a given time t , the stationary-phase condition for the energy integral in (30) reads $t = \hbar(d\bar{S}_\gamma/dE) = \bar{T}_\gamma$, so that only contributions of those paths $\gamma_{1 \rightarrow 1}$ whose (modified) orbiting time \bar{T}_γ equals t have to be taken into account. At least for short times, these are only a few paths, so that (28) provides a clear picture of the underlying dynamics. Care must be taken that the integration range in (29) and (30) does not exceed the range of validity of the path representation of G_E . In particular, the contributing energies have to be well above the highest of the minima of $V(x)$. This can be achieved by a suitable choice of the initial wavepacket Ψ_0 .

As an example, the dynamics of an initially Gaussian wavepacket in a double-minimum potential $V(x) = V_{\text{max}}[(x/x_0)^2 - 1]^2$ (see upper-right corner in figure 2(a)), centred at the leftmost turning point of energy $\bar{E} = V_{\text{max}}$ is considered. As the wavepacket evolves, each time it passes the barrier it splits into a transmitted and reflected part, so that after some time the resulting autocorrelation function shows complicated interference patterns (figure 2(a)). In figure 2(b) the square of the single contributions a_γ of some of the shortest paths $\gamma_{1 \rightarrow 1}$ are shown, neglecting any quantum mechanical interferences. With increasing length of the paths $\gamma_{1 \rightarrow 1}$, due to dispersion the contributions broaden. In figure 2(a) the square of the corresponding coherent sum (28) (full curve) together with a numerical evaluation of $a(t)$ based on a spectral representation ($H|n\rangle = E_n|n\rangle$)

$$a(t) = \sum_n |\langle n | \Psi_0 \rangle|^2 e^{-iE_n t/\hbar}$$

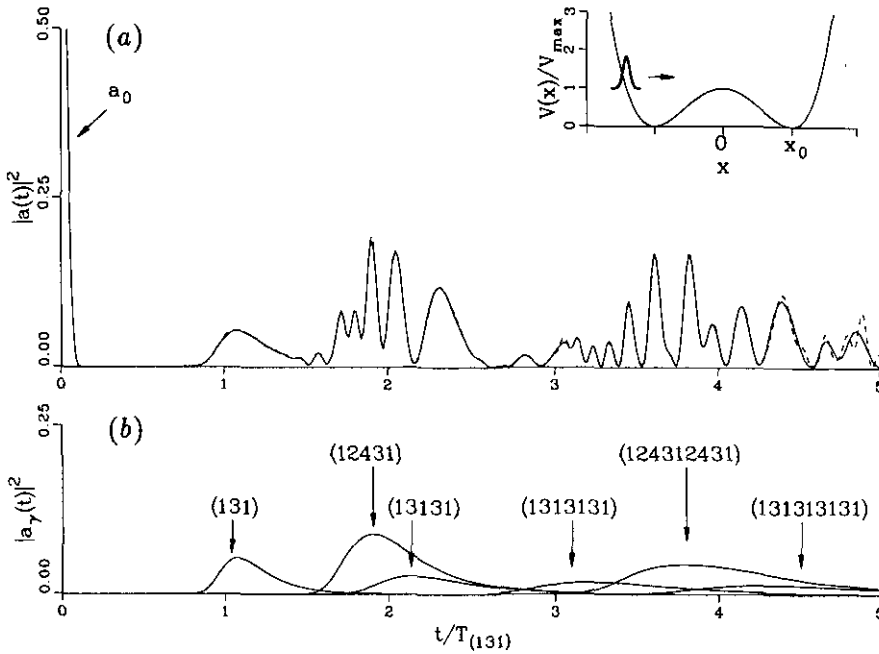


Figure 2. Square of the autocorrelation function $a(t)$ of a wavepacket in the double-minimum potential shown in the upper right corner. (a) Coherent sum (28) (full curve) and numerical evaluation of $a(t)$ (broken curve); (b) single contributions of the most important shortest paths.

(broken curve) is shown. With the help of figure 2(b), however, it is possible to identify peaks in $|a(t)|^2$ (figure 2(a)) as coherent superpositions of a small number of returning paths $\gamma_{l=1}^1$ of the wavepacket. In particular, the five-peak interference pattern around $t \approx 2T_{131}$ is due to the coherent superposition of the two contributions $a_{(12431)}$ and $a_{(13131)}$.

5.2. Quantization of disordered systems

In section 3 a closed-path representation (equations (15), (19)) of the density of states $d(E)$ in a multiple-well potential, valid for energies well above the minima of $V(x)$, is derived. It is especially useful whenever high frequencies (i.e. long cycles) are suppressed. This is the case for the density of states of a disordered potential, modelling disordered solids (liquid metals, amorphous substances, alloys) [10–12]. Here, for simplicity, the problem of *spatial* disorder is considered. This means that the potential $V(x)$ consists of identical barriers with random separations L_i (see upper-right corner of figure 3). It is assumed that the separations L_i are identically distributed independently, according to a Gaussian function with mean value L_0 and width σ ,

$$p(L_i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(1/2)[(L_i - L_0)/\sigma]^2}.$$

Here, the quantity of interest is the average density of states d_{av} [12] in the limit of an infinitely long chain of barriers as defined via

$$d_{av}(E) = \lim_{N \rightarrow \infty} \frac{\langle d(E) \rangle}{N}. \quad (31)$$

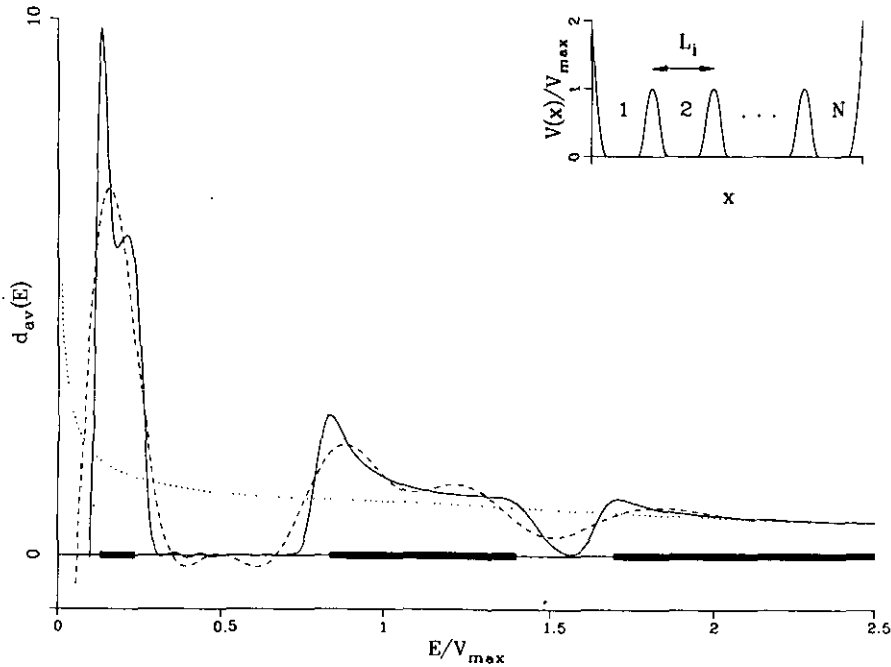


Figure 3. Average density of states $d_{av}(E)$ according to equation (32) for an infinite number of wells ($N \rightarrow \infty$) with disorder of five per cent. The dotted curve indicates $\bar{d}(E)$, the broken (full) curve includes all primitive cycles up to a length of 4 (20). The black bars indicate the positions of the allowed bands in the corresponding periodic ($\sigma = 0$) potential.

Taking the average reduces to evaluating Fourier transforms of Gaussian functions and can therefore be carried out analytically. To determine the density of states for fixed N , one has to sum over all primitive cycles of the graph. However, taking the average over the separations L_i means that the contribution of a specific cycle is independent of its position along the graph. All translated cycles of the same shape carry the same weight. Since their number divided by N tends to unity for large N , the summation over all primitive cycles and division by N in (31) may be replaced by a summation (\sum^*) over all translationally different primitive cycles. Therefore

$$d_{av}(E) = \frac{\bar{T}_0}{2\pi\hbar} + \frac{1}{\pi\hbar} \operatorname{Re} \left\{ \sum_{[\gamma^p]}^* \sum_{m=1}^{\infty} \tau_{\gamma} \Lambda_{\gamma}^m e^{im(\bar{S}_{\gamma} - m_{\gamma}\pi/2)} e^{-(1/2)(mn_{\gamma}k\sigma)^2} \right\} \quad (32)$$

where $\tau_{\gamma} = \bar{T}_{\gamma} - i\hbar[(\Lambda'_{\gamma}/\Lambda_{\gamma}) - m(n_{\gamma}k\sigma)^2]/(2E)$, $k = \sqrt{2\mu E}/\hbar$ is the wavenumber inside a well and n_{γ}^2 is the square sum of the numbers $n_{\gamma}^{(i)}$ of traversals through each well i , i.e. $n_{\gamma}^2 = \sum (n_{\gamma}^{(i)})^2$. The summation in (32) is extended over all primitive cycles which are different under translations (\sum^*) and their multiple repetitions m . Comparing with the corresponding result for the periodic ($\sigma = 0$) system, it is realized that introducing disorder essentially means suppressing long cycles exponentially with a factor $e^{-(1/2)(mn_{\gamma}k\sigma)^2}$. Therefore, in evaluating the sum in (32), only the shortest cycles (small m, n_{γ}) contribute significantly. Moreover, with growing disorder σ , fewer and fewer cycles $[\gamma^p]$ have to be taken into account.

As an example, in figure 3 the average density of states $d_{av}(E)$ in the case of five per cent disorder ($\sigma = 0.05L_0$) is shown. The barriers are piecewise parabolic (see upper-right corner in figure 3). The black bars indicate the positions of the allowed bands in the corresponding periodic ($\sigma = 0$) potential. The dotted curve shows $\bar{d}(E)$. The broken and full curves show $d_{av}(E)$ according to (32). For the broken curve, all cycles up to length 4 (contributions of 2(!) primitive cycles) are taken into account. The full curve shows (32) including all primitive cycles up to a length 20 (13 083 primitive cycles). Taking into account longer cycles does not change the results significantly.

6. Conclusion

In this paper a uniform semiclassical path representation of the energy-dependent Green function in a one-dimensional multiple-well potential has been derived. The key step is the replacement of the (2×2) transfer-matrices of semiclassical mechanics by a single $(2N \times 2N)$ matrix \mathcal{A} , characterizing the whole system. Interpreting \mathcal{A} as the weighted adjacency matrix of a graph, it has been shown that this approach provides a path representation of $G_E(x, x')$. The corresponding graph may be interpreted as the semiclassical phase-space portrait of the system. Based on this representation of $G_E(x, x')$, a closed-path representation of the density of states has been derived. Further, the semiclassical quantization condition may be expressed in terms of selected combinations of cycles of the graph (*permutation cycles*), generalizing the Bohr–Sommerfeld quantization applicable to the case $N = 1$.

Two applications, the semiclassical wavepacket autocorrelation function and the density of states of a disordered potential demonstrate the usefulness of this approach for different phenomena and for a wide range in the number of wells.

Appendix A. Results from uniform semiclassical mechanics

The uniform formulae for the barrier reflection coefficient and scattering phase shift can be found by mapping the barrier onto the inverse parabola [15, 1]. For energies $E < V_{\max} = V(x_{\max})$ one has two real turning points $x_>, x_<$. For energies $E > V_{\max}$, however, there are two complex-conjugate turning points x_+, x_- .

For $E > V_{\max}$, the real above-barrier reflection point x_r is implicitly defined via

$$\int_{x_r}^{x_{\max}} dx k(x) = \frac{1}{2} \left(\int_{x_+}^{x_{\max}} dz k(z) + \int_{x_-}^{x_{\max}} dz k(z) \right) \quad (\text{A1})$$

with (complex) wavenumber $k(z) = \sqrt{2m[E - V(z)]}/\hbar$.

The semiclassical reflection amplitude ρ and phase shift ϕ of a barrier are defined via the *tunnelling integral*

$$\epsilon(E) = \begin{cases} -\frac{1}{\pi} \int_{x_>}^{x_<} dx |k(x)| & \text{for } E \leq V_{\max} \\ -\frac{i}{\pi} \int_{x_+}^{x_-} dz k(z) & \text{for } E > V_{\max} \end{cases}$$

namely

$$\rho(E) = \frac{e^{-\pi\epsilon}}{\sqrt{1 + e^{-2\pi\epsilon}}} \quad (\text{A2})$$

and

$$\phi(E) = \arg\left[\Gamma\left(\frac{1}{2} + i\epsilon\right)\right] - \epsilon \ln|\epsilon| + \epsilon. \quad (\text{A3})$$

Appendix B. Basic graph-theoretical concepts

Basic definitions and concepts of graph theory may be found in [13,14]. A *finite, directed graph* $G = (V, E)$ consists of a set of vertices $V = \{1, \dots, n\}$ and a set of ordered pairs $E = \{(i, j), \dots\}$ the (*directed*) edges of the graph. A *path* $\gamma_{i \rightarrow j}$ of length m (written as $|\gamma_{i \rightarrow j}| = m$) which joins the vertices i and j is written as $\gamma_{i \rightarrow j} = (ik_1 \dots k_{m-1}j)$. The pairs $(i, k_1), (k_1, k_2), \dots, (k_{m-1}, j)$ have to be edges of the graph. Moreover, $\gamma_{i \rightarrow j}$ is called *closed*, if $i = j$.

A *weighted graph* is characterized by additional (complex) weights $w(i, j)$ of the edges (i, j) . It can be represented by its *weighted adjacency matrix* \mathcal{A} , which is defined via $\mathcal{A}_{ij} = w(i, j)$ if (i, j) is an edge of the graph. The matrix element \mathcal{A}_{ij} is set to zero if the edge (i, j) of the graph is missing. The common *adjacency matrix* used in elementary graph theory is given by unit weights, $w(i, j) = 1$ if $(i, j) \in E$. Finally, the weight $w(\gamma_{i \rightarrow j})$ of a *path* is the product of the weights of the edges of the path,

$$w(\gamma_{i \rightarrow j}) = w(i, k_1)w(k_1, k_2) \dots w(k_{m-1}, j).$$

The weighted adjacency matrix \mathcal{A} can be used to determine sums of weights of paths. Therefore, recall the definition of matrix-multiplication,

$$(\mathcal{A}^m)_{ij} = \sum_{k_1, \dots, k_{m-1}=1}^n \mathcal{A}_{ik_1} \mathcal{A}_{k_1 k_2} \dots \mathcal{A}_{k_{m-1} j}. \quad (\text{B1})$$

A summand in (B1) is non-zero only if the corresponding path $\gamma_{i \rightarrow j} = (ik_1 \dots k_{m-1}j)$ of length m exists in the graph. In this case the summand is equal to the weight of the path. Therefore,

$$(\mathcal{A}^m)_{ij} = \sum_{\substack{\gamma_{i \rightarrow j} \\ |\gamma_{i \rightarrow j}|=m}} w(\gamma_{i \rightarrow j}) \quad (\text{B2})$$

the summation being extended over all paths $\gamma_{i \rightarrow j}$ of length m . The sum of the weights of *all* paths $\gamma_{i \rightarrow j}$ is given by

$$\sum_{\gamma_{i \rightarrow j}} w(\gamma_{i \rightarrow j}) = \sum_{m=1}^{\infty} (\mathcal{A}^m)_{ij} = [(\mathbb{1} - \mathcal{A})^{-1}]_{ij} - \delta_{ij}. \quad (\text{B3})$$

In section 2 use is made of this equivalence to express the inverse of the matrix $(\mathbb{1} - \mathcal{A})$ as a sum over paths of the corresponding graph.

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