ISSN 0027-1349, Moscow University Physics Bulletin, 2007, Vol. 62, No. 4, pp. 210–215. © Allerton Press, Inc., 2007.
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Monte Carlo Method for the Schrödinger Equation with an Asymmetric Periodic Potential

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Received June 5, 2006

Abstract—A new numerical method is proposed for solving the Cauchy problem for the Schrödinger equation with an asymmetric periodic potential superimposed by a constant electric field. The solution to the Cauchy problem is used to determine the electron's mean momentum as a function of time, initial conditions, and the applied field. Given an initial state, the mean momentum characterizes the mean current and the conductivity of an asymmetric periodic structure known as the ratchet potential.

DOI: 10.3103/S0027134907040029

INTRODUCTION

The motion of particles in spatially periodic asymmetric systems (known as ratchets) attracted attention more than ten years ago as motivated by the interesting properties of these systems. Initially, the mechanism of ratchet systems was used to explain the transfer of certain substances in living cells (the theory of molecular motors); later, several engineering applications of this mechanism were proposed [1].

The theoretical study of this problem was complicated by the lack of a sufficiently reliable numerical algorithm even in the case of fairly simple models. In this paper, a quantum ratchet system is analyzed by applying a Monte Carlo technique [2–4]. Accordingly, no grids have to be constructed and the computational error can easily be estimated. The problem under study concerns the motion of an electron in the potential

$$V(x) = eEx + V_0 \sum_{k=1}^{K} \frac{\sin(kx)}{k}, \quad (1)$$

where the linear part describes the applied electric field and the superposition of harmonics produces an asymmetric periodic ratchet potential. The Fourier transform of this potential is a superposition of $2K$ Dirac functions at the points $\{\pm k\}_1^K$. Therefore, the Monte Carlo method can be reduced to the simulation of a homogeneous Poisson process representing a random walk with steps from the set $\{\pm k\}_1^K$. The linear part of the potential is taken into account by using the interaction representation.

SCHRÖDINGER EQUATION IN THE INTERACTION REPRESENTATION

Consider the Cauchy problem for the Schrödinger equation with the potential $v(y)$ given by (1):

$$i\hbar\frac{\partial\Psi}{\partial\tau} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} - f_\omega(\tau)x + v\left(\frac{y}{a}\right)\right)\Psi,$$
$$\Psi(y, 0) = \Psi_0(y), \quad v(y) = V_0\sum_{k=1}^{K}\frac{\sin\left(k\frac{2\pi y}{L}\right)}{k}, \quad (2)$$

where $L = 2\pi a$ and the force $f_\omega(\tau) = eE_\omega(\tau)$ is the electron charge times the strength of the superposition of the constant applied electric field and the random component corresponding to the interaction of conduction electrons with the medium (ω is a random parameter).

After we introduce the new dimensionless variables $t = \frac{\hbar}{ma^2}\tau$ and $x = \frac{y}{a}$ and make the substitutions

$$\tau \longrightarrow t, \quad y \longrightarrow x, \quad \Psi(y, \tau) \longrightarrow \psi(x, t),$$
$$v(y) \longrightarrow V(x) = \frac{ma^2}{\hbar^2}v(ax),$$
$$f_\omega(\tau) \longrightarrow F_\omega(t) = \frac{ma^3}{\hbar^2}f_\omega\left(\frac{ma^2}{\hbar}\tau\right).$$

Equation (2) becomes

$$i\frac{\partial\psi(x, t)}{\partial t} = (\hat{H}_0 + V(x))\psi(x, t),$$
$$\psi(x, 0) = \psi_0(x) = \Psi_0(ax), \quad \hat{H}_0 = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - F_\omega(t)x. \quad (3)$$

The function $V(x)$ can be represented as the Fourier transform of a complex-valued Radon measure with a finite variation [2]:

$$V(x) = \kappa\int_{\mathbb{R}}\mu(dq)e^{-iqx+i\alpha(q)}$$

$$= V_0\sum_{k=1}^{K}\frac{1}{2k}\int_{\mathbb{R}} dq e^{-iqx}\left(e^{i\frac{\pi}{2}}\delta(q-k) + e^{-i\frac{\pi}{2}}\delta(q+k)\right),$$

where $\kappa = V_0\sum_{k=1}^{K}\frac{1}{k}$. To proceed to the momentum representation, we use the Fourier transform $\mathcal{F}_{x\to p}\varphi(x) = \tilde{\varphi}(p) = \frac{1}{\sqrt{2\pi}}\int e^{-ipx}\varphi(x)dx$. Denote by $U_{0,t}$ the unitary cocycle $U_{0,t} = \overrightarrow{e}^{i\int_0^t \hat{H}_0(s)ds}$ written as a chronological exponential, so that $\frac{d}{dt}U_{0,t} = iU_{0,t}\hat{H}_0(t)$. This cocycle has the commutation properties

$$\hat{p}_t = U_{0,t}\hat{p}U_{0,t}^* = \hat{p} + P_\omega(t),$$

$$P_\omega(t) = \int_0^t F_\omega(s)ds,$$

$$\hat{x}_t = U_{0,t}\hat{x}U_{0,t}^* = \hat{x} + \hat{p}t + X_\omega(t),$$

$$X_\omega(t) = \int_0^t P_\omega(s)ds.$$

Applying the Baker–Hausdorff formula yields the following expression for $\hat{V}_t$ in the momentum representation:

$$\hat{V}_t = U_{0,t}V(\hat{x})U_{0,t}^* = \kappa\int_{\mathbb{R}}\mu(dq)e^{-iq\hat{x}_t + i\alpha(q)}$$

$$= \kappa\int_{\mathbb{R}}\mu(dq)e^{i\left(-\frac{1}{2}q^2t - qX_\omega(t) + \alpha(q) - qpt\right)}e^{q\frac{\partial}{\partial p}}.$$

Note that, if $\psi(x, t)$ is a solution to Eq. (3), then the Schrödinger equation for $\tilde{\varphi}(p, t) = e^{-\kappa t}\mathcal{F}_{x\to p}U_{0,t}\psi(x, t)$ can be written as the expectation of a superposition of exponentials of the stochastic action S:

$$\frac{\partial\tilde{\varphi}(p,t)}{\partial t} = \left(\frac{1}{i}\hat{V}_t - \kappa\right)\tilde{\varphi}(p,t)$$
$$= \kappa\int_{\mathbb{R}}\mu(dq)(e^{iS(p,q,t)}\tilde{\varphi}(p+q,t) - \tilde{\varphi}(p,t)), \tag{4}$$

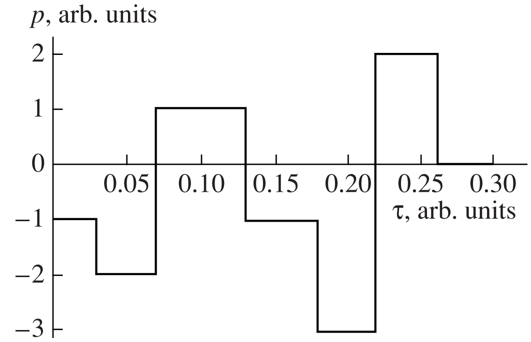

Fig. 1. Example of a Markov jump process.

$$S(p,q,t) = -\frac{1}{2}q^2t - qX_\omega(t) + \alpha(q) - \frac{\pi}{2} - qpt,$$
$$\tilde{\varphi}(p,0) = \tilde{\psi}_0(p). \tag{5}$$

By the Duhamel principle, this equation is equivalent to the integral equation

$$\tilde{\varphi}(p,t) = e^{-\kappa t}\tilde{\psi}_0(p)$$
$$+ \kappa\int_0^t d\tau e^{-(t-\tau)\kappa}\int_{\mathbb{R}}\mu(dq)\tilde{\varphi}(p+q,\tau)e^{iS(p,q,\tau)},$$

whose solution can be written as an absolutely convergent series

$$\tilde{\varphi}(p,t) = e^{-\kappa t}\Bigg\{\tilde{\psi}_0(p) + \sum_{n=1}^{\infty}\kappa^n\int_0^t\ldots\int_0^{t_{n-1}}dt_1$$
$$\times\ldots dt_n\int_{\mathbb{R}}\mu(dq_1)\ldots\int_{\mathbb{R}}\mu(dq_n)\tilde{\psi}_0\left(p + \sum_{k=1}^{n}q_k\right) \tag{6}$$
$$\times\exp\left(i\sum_{k=1}^{n}S\left(p + \sum_{j=0}^{k-1}q_j, q_k, t_k\right)\right)\Bigg\}.$$

NUMERICAL IMPLEMENTATION OF THE MONTE CARLO METHOD

To implement the Monte Carlo method numerically, we consider a Markov jump process starting at the point $p(t) = 0$ at time $t = \tau$ and going back to the time $\tau = 0$ (see Fig. 1). Let $p_n = p(t_n) = \sum_{j=0}^{n}q_j$ be the current momentum of the path after n jumps, q_j be the size of the jth jump, $t_n = t - \sum_{j=0}^{n}\tau_j$ be the time of the nth jump, τ_j be the random waiting time of the jth jump, and

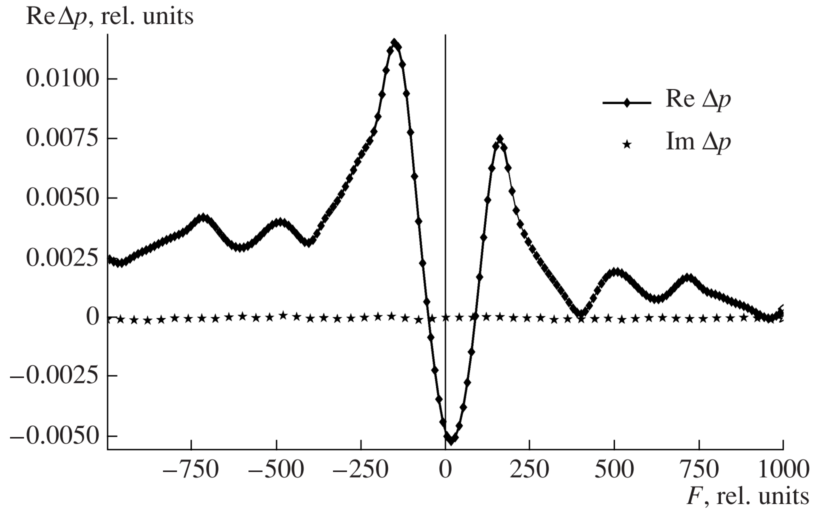

Fig. 2. Typical function $\Delta p(F)$ at $x_0 = 0$.

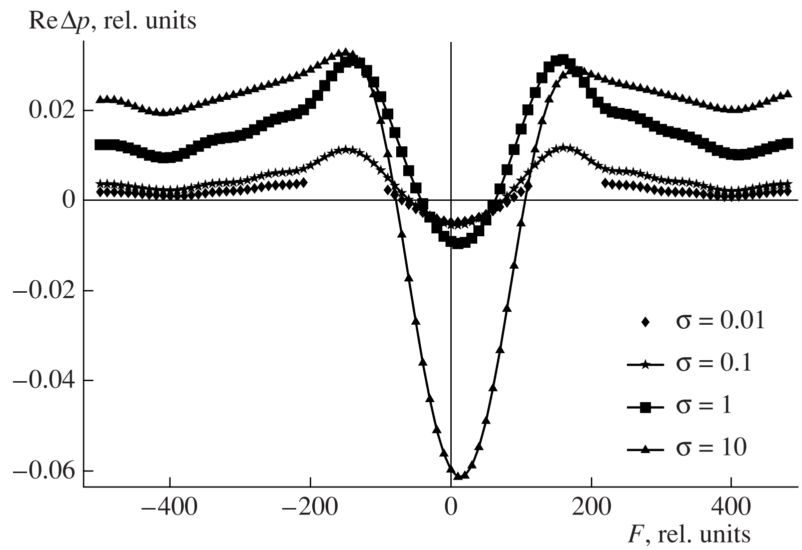

Fig. 3. Dependence Re$\Delta p(F)$ for various σ at $x_0 = 0$.

$$\mathbb{P}\{q_j = \pm n\} = \frac{1}{2}\frac{n^{-1}}{\sum_1^K k^{-1}},$$

$$\mathbb{P}\{\tau_j > T\} = e^{-\kappa T}, \quad \kappa = V_0\sum_{k=1}^K k^{-1}$$

for any j. This jump process is homogeneous in the momentum space and with respect to time. It can be shown that the sum of series (6) can be equivalently represented as the expectation of a functional defined on paths of a homogeneous Poisson process [2–5]:

$$\tilde{\varphi}(p, t) = \mathbb{M}_t\tilde{\psi}_0(p + p_N) \times \exp\left(i\sum_{n=0}^N S(p + p_{n-1}, q_n, t_n)\right),$$

where $N = N(t)$ is the random number of jumps along the path $p(\tau)$. The momentum variation Δp_t caused by the quantum interaction with the ratchet potential can be represented as

$$\Delta p_t = e^{2\kappa t}\int_{\mathbb{R}}\tilde{\varphi}^*(p, t)\hat{p}\tilde{\varphi}(p, t)dp.$$

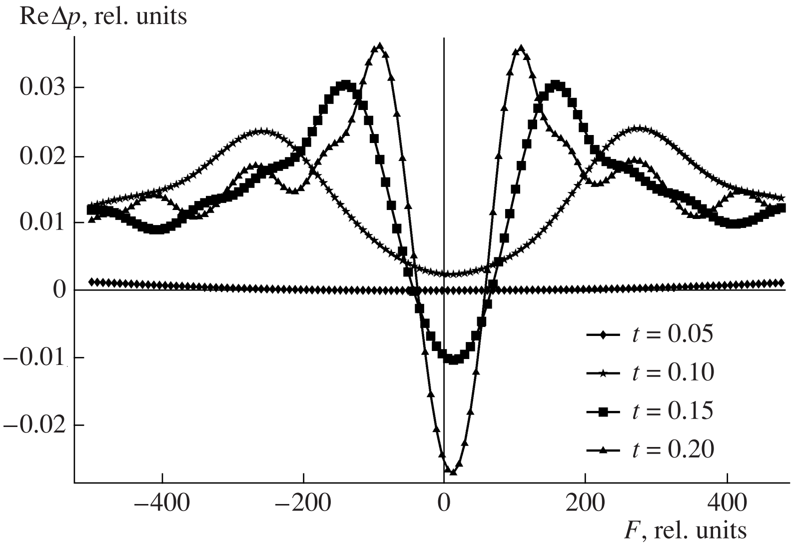

Fig. 4. Dependence $\mathrm{Re}\Delta p(F)$ for various t at $x_0 = 0$.

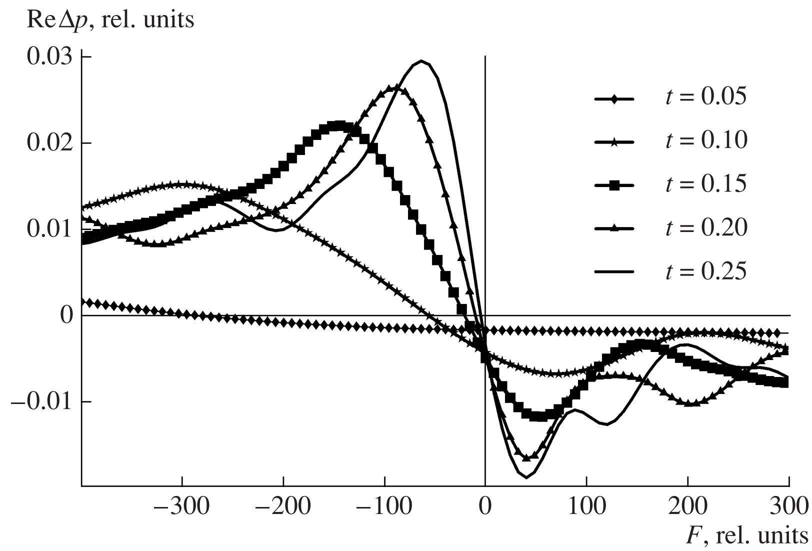

Fig. 5. Dependence $\mathrm{Re}\Delta p(F)$ for various t at $x_0 = 1$.

To simplify the algorithmization of the Monte Carlo method, it is convenient to represent the solution to the Cauchy problem for Eq. (4) in the form

$$\tilde{\varphi}(p, t) = \mathbb{M}_t e^{iA - iBp} \tilde{\psi}_0(p + C),$$

$$A = -\sum_{k=1}^{N} \left(\frac{1}{2} q_k^2 t_k + q_k X_\omega(t_k) - \alpha(q_k) + \frac{\pi}{2} + q_k t_k \sum_{j=1}^{k-1} q_j \right),$$

$$B = \sum_{k=1}^{N} q_k t_k, \quad C = \sum_{k=1}^{N} q_k.$$

The double randomization principle implies that

$$\Delta p_t = e^{2\kappa t} \mathbb{M}_t e^{i(A_1 - A_2)} R(B_1 - B_2, C_1, C_2),$$

$$R(B, C_1, C_2) = \int_{\mathbb{R}} p e^{-iBp} \tilde{\varphi}_0^*(p + C_2) \tilde{\varphi}_0(p + C_1) dp,$$

where A_1, B_1, C_1 and A_2, B_2, C_2 are random variables (functionals of random paths) corresponding to two independent paths of the Markov jump process described above.

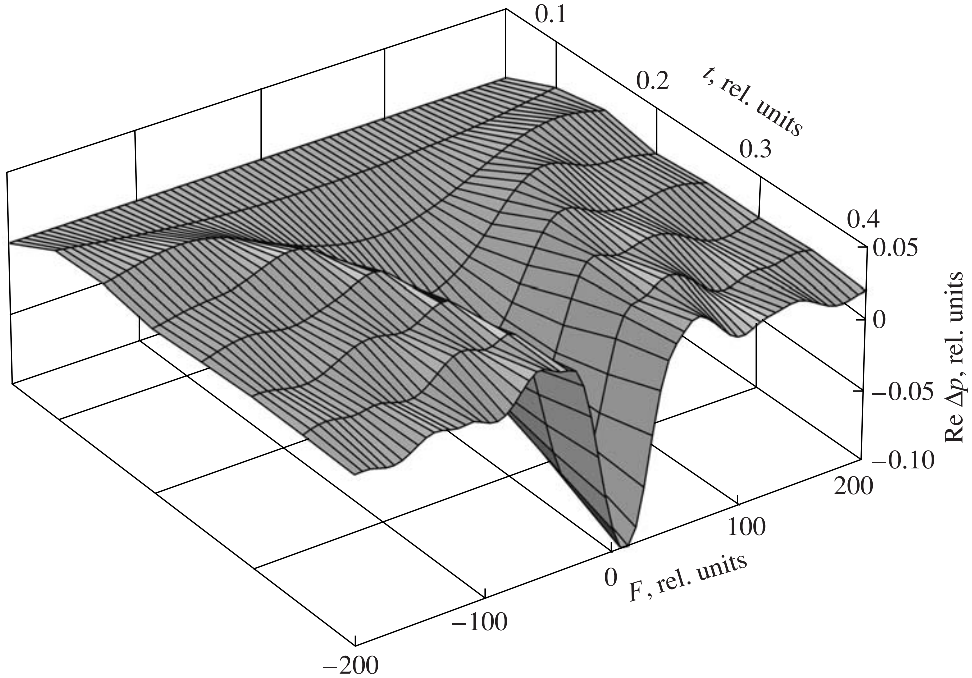

Fig. 6. Dependence Re$\Delta p(F, t)$ at $x_0 = 0$.

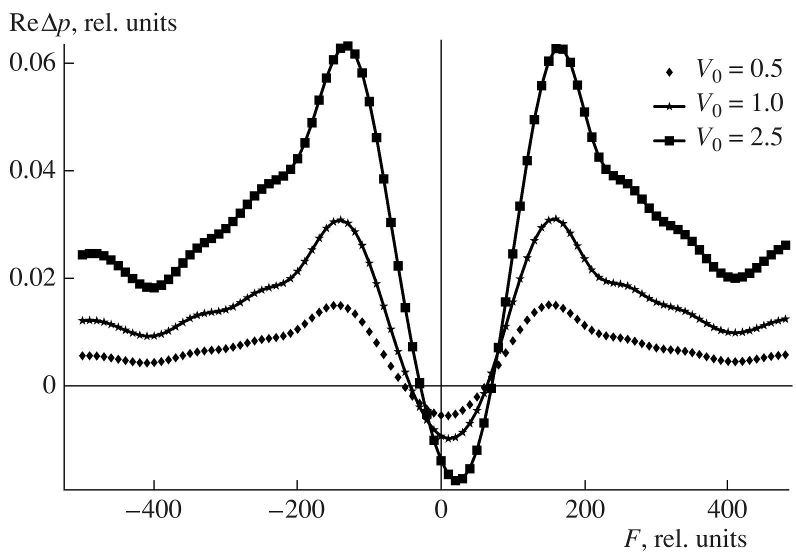

Fig. 7. Dependence Re$\Delta p(F)$ for various V_0 at $x_0 = 0$.

In the case of the Gaussian initial condition

$$\tilde{\varphi}_0(p) = \frac{1}{\sqrt[4]{2\pi\sigma}}\exp\left\{-\frac{(p-p_0)^2}{4\sigma} - ix_0p\right\},$$

$R(B, C_1, C_2)$ is explicitly determined as

$$R(B, C_1, C_2) = -\frac{1}{2}e^{\Phi(B, C_1, C_2)}(C_1 + C_2 - 2p_0 + 2iB\sigma),$$

where $\Phi(B, C_1, C_2) = -\frac{1}{8\sigma}(4B^2\sigma^2 + 4iB\sigma(C_1 + C_2 - 2p_0) + (C_1 - C_2)(C_1 - C_2 + 8ix_0\sigma))$.

It can be shown that the expectation of Δp_t converges at a rate proportional to $\frac{e^{\kappa t}}{\sqrt{N}}$. In practice, the computational error can be roughly estimated by the imaginary part of the sample mean momentum, which vanishes as $N \longrightarrow \infty$.

NUMERICAL RESULTS

The ratchet potential was simulated by the function $V(x) = V_0 \sum_{k=1}^{8} \frac{\sin(kx)}{k}$. The mean momenta of electrons interacting with the ratchet potential were estimated using up to $N = 10^9$ pairs of random paths. In all the numerical experiments, $F_\omega(t)$ was set equal to a constant value F.

The basic properties of the solution to the Cauchy problem for the Schrödinger equation, which can be observed by inspecting numerical approximations to the solution, are presented as plots. Note that Δp_t (or, up to a factor, the mean current ΔI_t) is a nonmonotonic function of the applied field and exhibits a series of maxima whose amplitudes decrease with increasing applied field. Figures 2–7 clearly reveal that this dependence is asymmetric about the direction of the applied field and the mean momentum is nonzero in the absence of the field. Figure 2 also shows the imaginary part of the momentum ($\mathrm{Im}\Delta p$), which gives an estimate of the computational error.

Figure 3 displays the mean momentum as a function of the applied field for various values of σ. These plots show that the contribution of the ratchet potential to the mean current increases as the packet width in the coordinate representation narrows.

Figures 4–6 show the mean current as a function of time and the applied field for various values of x_0. It can be seen that the maximum current increases with time and is reached at lower field values.

Figure 7 shows $\mathrm{Re}\Delta p(F)$ for various amplitudes of the ratchet potential. The plots suggest that the current increases monotonically with V_0.

CONCLUSIONS

Note that we considered only mathematical aspects of the method for solving the Cauchy problem for the Schrödinger equation with a periodic asymmetric potential. A discussion of whether or not the Brownian motor theory agrees with the second law of thermodynamics lies beyond the scope of this paper. In particular, we do not estimate the energy and entropy changes required for creating the initial Gaussian state $\rho_0 = |\psi_0\rangle\langle\psi_0|$ with a zero momentum and a large variance in the coordinate representation, for which the numerical experiment suggests the creation of the current ΔI_t. Possibly, the interaction of conduction electrons with Brownian surroundings is the mechanism that produces states close to ρ_0.

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