Application of the Wigner-Function Formulation to Mesoscopic Systems in Presence of Electron-Phonon Interaction

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July 21, 1997

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19971112 082

Abstract

A theoretical and computational analysis of the quantum dynamics of charge carriers in presence of electron-phonon interaction based on the Wigner function is here applied to the study of transport in mesoscopic systems. Numerical applications are shown for a) a wave packet scattering with phonons while crossing a potential profile and b) electrons scattering with phonons in a finite device with open boundary conditions.

Keywords: Quantum Transport, Wigner Function, Mesoscopic Systems, Boundary Conditions

1 Introduction

A rigorous quantum transport theory of electrons in semiconductor structures including both coherent propagation and scattering mechanisms is still lacking even though its need has been recognized since many years. In particular we miss a theory feasible for numerical calculations to be compared with experimental results and/or with results of the semiclassical theory with the purpose of enlightening the different predictions of the two models.

In the literature different approches have been used [1, 2, 3]. The Wigner function (WF) [1] provides a rigorous quantum-mechanical tool and constitues a direct link between quantum and classical descriptions of the evolution of the system in phase. In this approach however electron-phonon interaction has been treated using either relaxation time [4, 5] or a classical Boltzmann collision operator [6]. In this paper several advancements in the efford to solve the above problem exactly are presented.

The definition of the WF can be extended to include electrons interacting with phonons as follows [7]:

$$f_w(\mathbf{r}, \mathbf{p}, n_q, n'_q, t) = \frac{1}{h^3} \int d\mathbf{r}' e^{-i\frac{\mathbf{p}}{\hbar}\mathbf{r}'} \rho(\mathbf{r} + \mathbf{r}'/2, n_q; \mathbf{r} - \mathbf{r}'/2, n'_q) \tag{1}$$

where $\mathbf{r}$ and $\mathbf{p}$ are the electron position and momentum, ρ is the density matrix for the system formed by an electron and the phonon gas, and n_q is the occupation number of the phonon mode $\mathbf{q}$. Trace over the phonon variables will lead to the traditional electron WF.

In this paper we discuss an integral equation for the above WF and apply it to study quantum electron transport in open systems in presence of scattering. In particular suitable boundary conditions can be used which restrict the analysis of the WF inside a finite domain. Wigner trajectories have been identified also for the case of electron-phonon interaction and constitute a guiding criterion for replacing initial conditions with boundary conditions for the integral equation.

2 Integral Equation

Let us consider a system described by the Hamiltonian

$$\mathbf{H} = \mathbf{H}_\circ + \mathbf{H}' \tag{2}$$

where $\mathbf{H}_\circ$ is the "unperturbed" Hamiltonian, containing the description of the free electrons, free phonons and, in the present approach, also the potential profile inside the system (device). $\mathbf{H}'$ contains the scattering agents, i.e. the electron-phonon interaction.

The time evolution of the density matrix is described by the Liouville-von Neumann equation. Starting from this equation we derived the following integral equation for the WF:

$$\begin{aligned} f_w(\mathbf{r},\mathbf{p},n_q,n_q',t) &= h^3 \sum_{n,n'} f_{nn'}(\mathbf{r},\mathbf{p}) e^{-i(\omega(n,n_q)-\omega(n',n_q'))(t-t_\circ)} \int d\mathbf{r}' \int d\mathbf{p}' f^*_{nn'}(\mathbf{r}',\mathbf{p}') \\ &\times f_w(\mathbf{r}',\mathbf{p}',n_q,n_q',t_\circ) + h^3 \sum_{n,n'} f_{nn'}(\mathbf{r},\mathbf{p}) \int_{t_\circ}^{t} dt' e^{-i(\omega(n,n_q)-\omega(n',n_q'))(t-t')} \\ &\times \sum_{mm_q} \int d\mathbf{r}' \int d\mathbf{p}' \left\{ \mathcal{H}'(nn_q,mm_q) f^*_{mn'}(\mathbf{r}',\mathbf{p}') f_w(\mathbf{r}',\mathbf{p}',m_q,n_q',t') \right. \\ &\left. - f^*_{nm}(\mathbf{r}',\mathbf{p}') f_w(\mathbf{r}',\mathbf{p}',n_q,m_q,t') \mathcal{H}'(mm_q,n'n_q') \right\} \end{aligned} \tag{3}$$

In the above equation $\mathcal{H}' = \mathbf{H}'/i\hbar$, and $\mathcal{H}'(nn_q,mm_q)$ are its matrix elements on the basis $\{|\phi_l,n_q>\}$ of $\mathbf{H}_\circ$. The coefficients $f_{lm}(\mathbf{r},\mathbf{p})$ are given by

$$f_{lm}(\mathbf{r},\mathbf{p}) = \frac{1}{h^3} \int d\mathbf{r}' e^{-i\frac{\mathbf{p}}{\hbar}\mathbf{r}'} < \mathbf{r} + \frac{\mathbf{r}'}{2} |\phi_l >< \phi_m| \mathbf{r} - \frac{\mathbf{r}'}{2} > \tag{4}$$

They allow to move from the WF to the density-matrix representation and viceversa. Finally $\hbar\omega(n,n_q)$ indicates the total unperturbed energy of the electron-phonon system when the electron is in the n-th eigenstate and the phonon bath is in a state with n phonons in mode $\mathbf{q}$.

In Eq. 3 the first term in the r.h.s. describes the ballistic coherent propagation from the initial time $t_\circ$ to the observation time t. The second term describes the contribution of the unknown WF to the "last" interaction vertex at any time t' between $t_\circ$ and t followed by the free propagation from t' to t. Even though the equation is written for the entire system and

contains also the phonon variables, it has been shown that a Monte Carlo solution allows for a proper average over the phonon coordinates, as long as hot-phonon effects are neglected [8].

3 Wigner Trajectories

It is well known that a point-like electronic WF in phase space cannot represent a real physical system, since it violates the uncertainty principle. We may however consider the evolution in time of a $\delta-$like contribution to the WF inside Eq. 3. For free electrons its trajectory in phase space is the same as for semiclassical particles. In fact, for a plane-wave basis the coefficients f_{lm} are given by

$$f_{kk'}(\mathbf{r},\mathbf{p}) = \frac{1}{(2\pi)^3} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}} \delta^3(\mathbf{p} - \frac{\hbar}{2}(\mathbf{k}+\mathbf{k}')) \tag{5}$$

and the ballistic evolution of the WF as given by the first term on the rhs of Eq.3 yields:

$$f_w(\mathbf{r},\mathbf{p},n_q,n'_q,t) = f_w(\mathbf{r} - \frac{\mathbf{p}}{m}(t-t_\circ),\mathbf{p},n_q,n'_q,t_\circ) e^{-i(\omega(n_q)-\omega(n'_q))(t-t_\circ)} \tag{6}$$

where m is the electron effective mass. The first factor and the exponential factor describe the free trajectory of the electron and the time evolution of the free-phonon bath, respectively.

This result is not surprising since in absence of scattering and up to quadratic potentials (harmonic oscillator) a differential equation can be written for the WF that coincides with the Boltzmann equation, so that the dynamical evolution of the WF follows the same trajectories of the representative points of a classical gas. This implies a deformation of the WF while evolving in time due to the fact that, as time increases, the higher-momentum components move faster than the lower-momentum components.

If phonon scattering is included, similar trajectories exist, with very interesting properties, as long as a single interaction diagram is considered without time integrations. In order to prove this result Eq. 3 must be substituted into itself to obtain the second-order term corresponding to one scattering event. Then assuming a constant potential and using again plane waves as basis

set, the second-order correction, e.g. for the terms corresponding to phonon emission, results to be

$$\Delta f_w(z,p_z,n_q,n_q,t) = 2\Re\Big\{\sum_q F^2(q) < n_q > \int_{t_\circ}^{t} dt' \int_{t_\circ}^{t'} dt''\, e^{-iq\frac{p_z+\hbar q/2}{m}(t'-t'')} e^{i\omega_q(t'-t'')}$$
$$\times f_w(z-\tfrac{p_z}{m}(t-t') - \tfrac{p_z+\hbar q/2}{m}(t'-t'') - \tfrac{p_z+\hbar q}{m}(t''-t_\circ), p_z+\hbar q, n_q-1, n_q-1, t_\circ)\Big\} \quad (7)$$

where for simplicity a one-dimensional case is considered and $F(q)$ is the coupling function entering the electron-phonon hamiltonian [9]. The trajectories described by the above equation are represented in the diagrams contained in Fig. 1. They correspond to the semiclassical trajectories where $q/2$ is transferred to the electron at each vertex. As a result of the time integrations, however, a sum over infinite trajectories gives the WF correction corresponding to a single scattering event.

4 Initial and Boundary Conditions

Guided by the considerations of the previous section we face the problem of finding an equation equivalent to Eq. 3 for the WF in a finite region inside given boundaries. The problem is not trivial owing to the nonlocality of the interaction and to the integration from $-\infty$ to $+\infty$ in the integral over z'. We have proved that for the solution of the integral equation it is possible to substitute the knowledge of the WF over all space at a given (initial) time $t_\circ$ with the knowledge of the same function inside the region of interest at $t_\circ$ and at all times at the boundary for "entering" momenta. The integral equation for such a situation results to be

$$f_w\left(z,p_z,n_q,n_q',t\right) =$$
$$h\sum_{nn'} f_{nn'}(z,p_z)\, e^{-i\left(\omega(nn_q)-\omega(n'n_q')\right)(t-t_\circ)} \int_{-A}^{A} dz' \int dp_z' f_{nn'}^*(z',p_z')\, f_w\left(z',p_z',n_q,n_q',t_\circ\right)$$
$$+h\sum_{nn'} f_{nn'}(z,p_z) \int_{t_\circ}^{t} dt'\, e^{-i\left(\omega(nn_q)-\omega(n'n_q')\right)(t-t')} \Big\{\Big[\int_0^{+\infty} dp_z' \frac{p_z'}{m} f_{nn'}^*(-A,p_z')$$
$$\times f_w\left(-A,p_z',n_q,n_q',t'\right) - \int_{-\infty}^{0} dp_z' \frac{p_z'}{m} f_{nn'}^*(A,p_z')\, f_w\left(A,p_z',n_q,n_q',t'\right)\Big]$$

$$+\int_{-A}^{A} dz' \int dp'_z \sum_{mm_q} \left[\mathcal{H}'(nn_q, mm_q)\, f^*_{mn'}(z', p'_z)\, f_w\left(z', p'_z, m_q, n'_q, t'\right)\right.$$

$$\left.-f^*_{nm}(z', p'_z)\, f_w(z', p'_z, n_q, m_q, t')\, \mathcal{H}'\left(mm_q, n'n'_q\right)\right]\Big\}. \tag{8}$$

where again for simplicity a one-dimensional case has been considered, and $-A$ and A are the device boundaries.

5 Applications

As a case study we have first analysed a single electron-phonon scattering event for a wave packet crossing a potential profile [10]. In this case the numerical procedure is simplified by the fact that the whole system can be enclosed in a large, but finite box. Thus the basis set of functions is discrete and can be used without finite-difference approximations in **k**-space. Three cases have been considered for a single electron-phonon scattering event: a) the effect of a quantum collision over the free propagation, b) intra-collisional field effect when the phonon interaction takes place during a propagation through a region with a constant electric field, and c) scattering during the otherwise resonant propagation through a double barrier. As an example Fig. 2 shows the scattering and scattered WF at $t = 1.5ps$ after the initial condition for an electron crossing a double barrier in resonant conditions and emitting an optical phonon. The interaction is switched on when the packet hits the double barrier, namely at $t = 0.5ps$ after the initial condition. A complex quantum-dynamical interference between potential profile and scattering is observed at successive times [10].

In order to verify the correctness of the use of the boundary conditions for an open mesoscopic system as described in Section 4 we have first evaluated the ballistic evolution of the first term in Eq.8 assuming a step potential profile, $f_w = 0$ at $t = t_o$ inside the device, and a Maxwellian local-equilibrium incoming distribution at the left and right boundaries. Results are shown in Fig. 3 at different times after the initial condition.

At the longest times (not shown in the figure for space reasons) we recover for f_w the same result which is obtained without using boundary conditions for a stationary infinite system, where f_w is evaluated by means of an equilibrium density matrix diagonal over the scattering states.

In order to describe quantum transport across a very small device in presence of scattering the integral Eq.8 is expanded perturbatively through iterative substitutions. The second-order contribution is the sum of four terms: real and virtual absorptions and emissions. As an example Fig. 4 shows the result for the in-emission term summed over all phonon modes q which compares very well with the classical result.

An interesting difference instead emerges when only a single mode q is considered in the quantum calculation, as shown in Fig. 5. At short times right after the entrance energy non-conservation modifies the in-scattering term.

Partially supported by ARO and ONR through ERO through Contract n. N68171-96-C-9089.

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6 Biographies

Carlo Jacoboni(Ph.D. in Physics at Purdue University, Indiana, in 1969) is Full Professor of Theoretical Physics and Dean of the Faculty of Sciences. **Antonio Abramo** (Ph.D. in Electrical Engineering at the University of Bologna, Italy in 1995) is Post-Doc at the University of Modena. **Paolo Bordone** (Ph.D. in Physics at the University of Modena, Italy in 1992) is Post-Doc at the University of Modena. **Rossella Brunetti** (Ph.D. in Physics at the University of Modena, Italy in 1987) is Research and Teaching Assistant at the Physics Department of the University of Modena. **Marco Pascoli** (Laurea in Physics at the University of Modena, Italy in 1996). The research activity of the group is mainly related to Monte Carlo applications to semiclassical and quantum transport and electron-device modeling.

Figure 1: Example of the Wigner trajectories that contribute to the result in Eq. 3 for real and virtual emissions of a mode q.

Figure 2: Unperturbed Wigner function (above) and second-order correction due to a quantum phonon emission (below) for an electron crossing a double-barrier potential profile in resonant conditions at different times. The interaction is active from $t = 0.5$ ps after the initial condition.

Figure 3: Ballistic evolution of the first term in Eq. (8) at d times ($t = 10$ fs and $80fs$) for electrons entering from the boundaries into a region with a potential step.

Figure 4: In-emission term summed over all phonon modes q at $t = 50$ fs after the electron-phonon interaction has been switched on.

Figure 5: Contribution to the Wigner function due to real emission of a mode $q = 1.66 \cdot 10^8$ m^{-1} at $200fs$ after the electron-phonon interaction has been switched on. Only electrons entering with positive p are able to emit. At long times classical conservation is recovered.

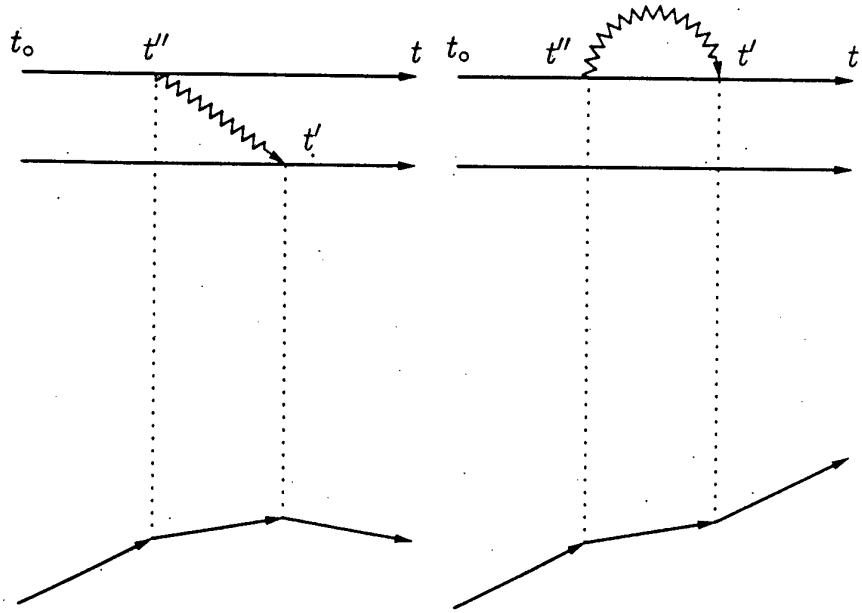


Fig. 2

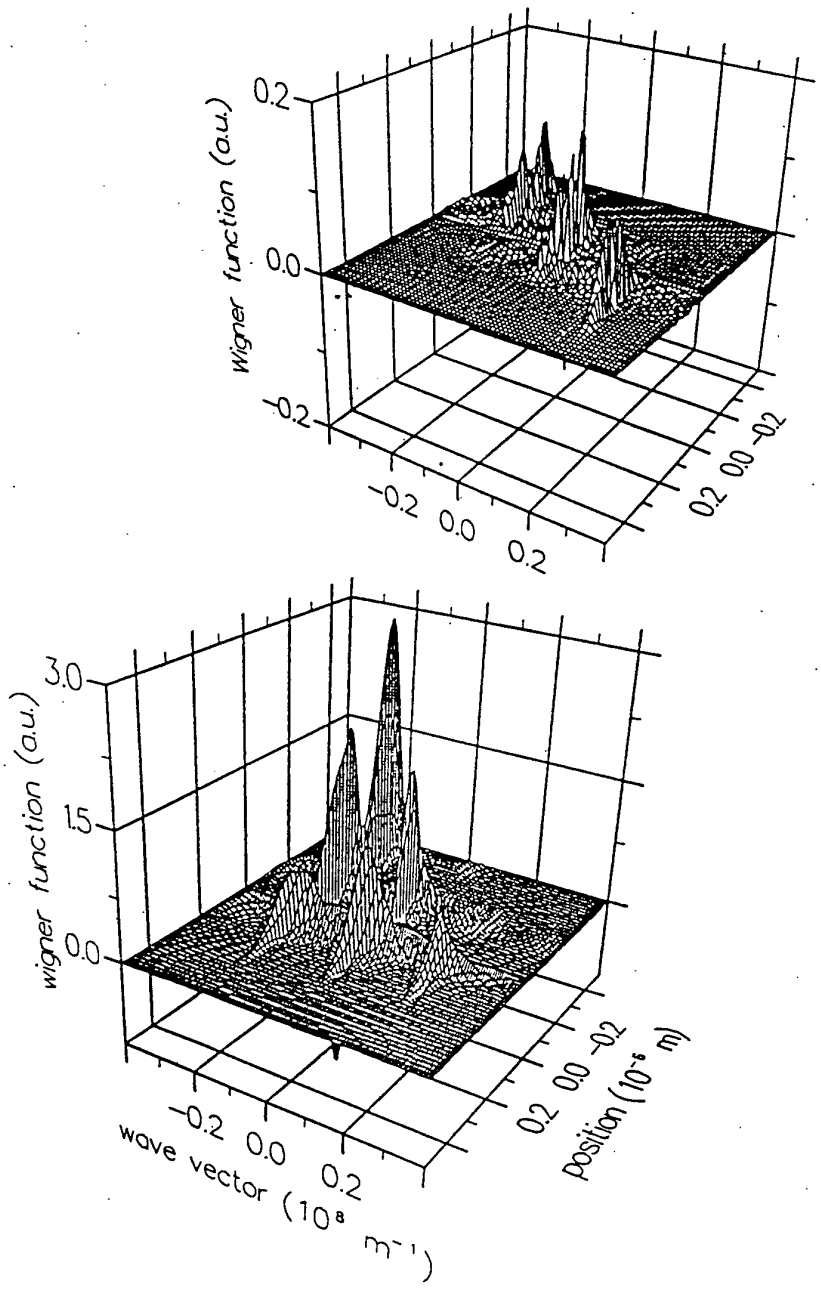
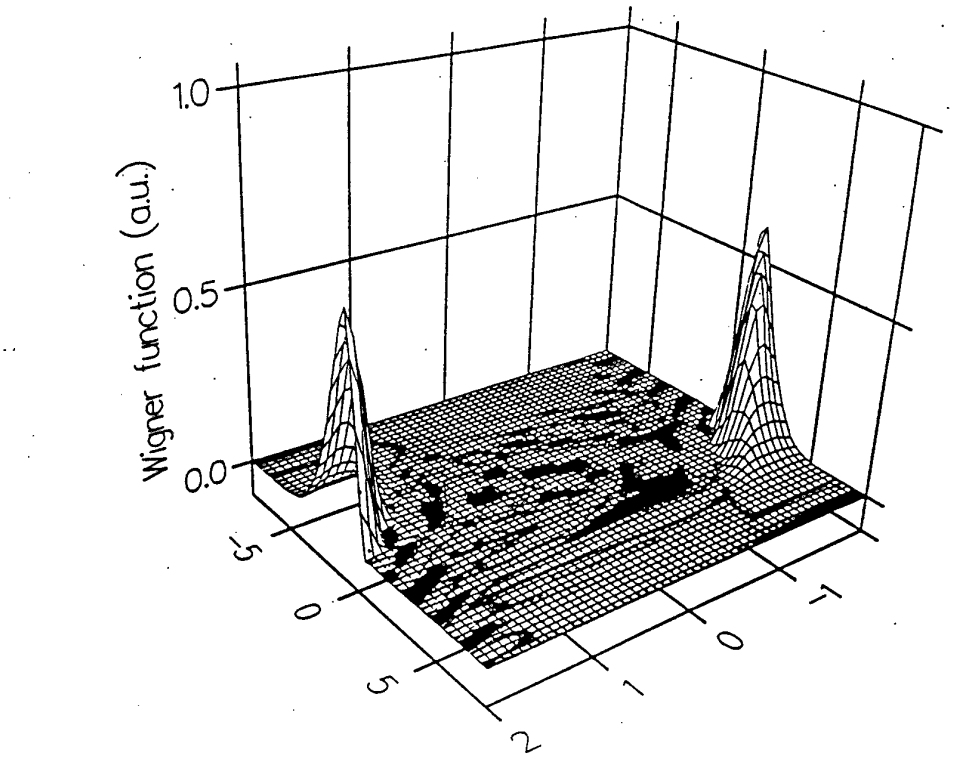
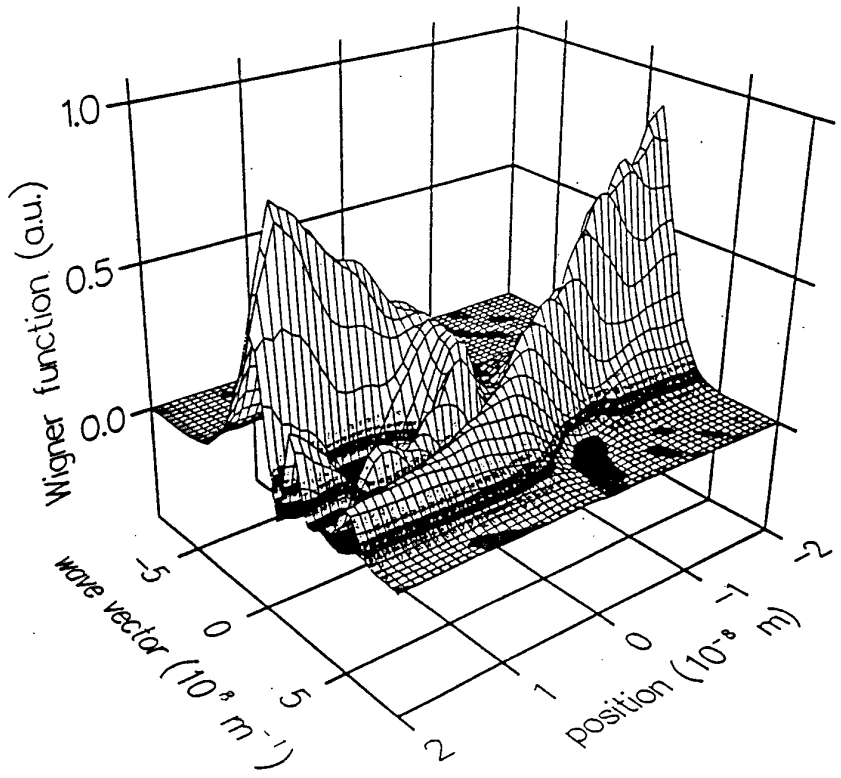

Wigner function (a.u.)
0.2
0.0
-0.2
-0.2 0.0 0.2
0.2 0.0 -0.2
wigner function (a.u.)
3.0
1.5
0.0
-0.2 0.0 0.2
wave vector (10⁸ m⁻¹)
0.2 0.0 -0.2
position (10⁻⁶ m)

Fig. 2


1.0
0.5
0.0
Wigner function (a.u.)
-5
0
5
2
1
0
-1


1.0
0.5
0.0
Wigner function (a.u.)
wave vector (10⁸ m⁻¹)
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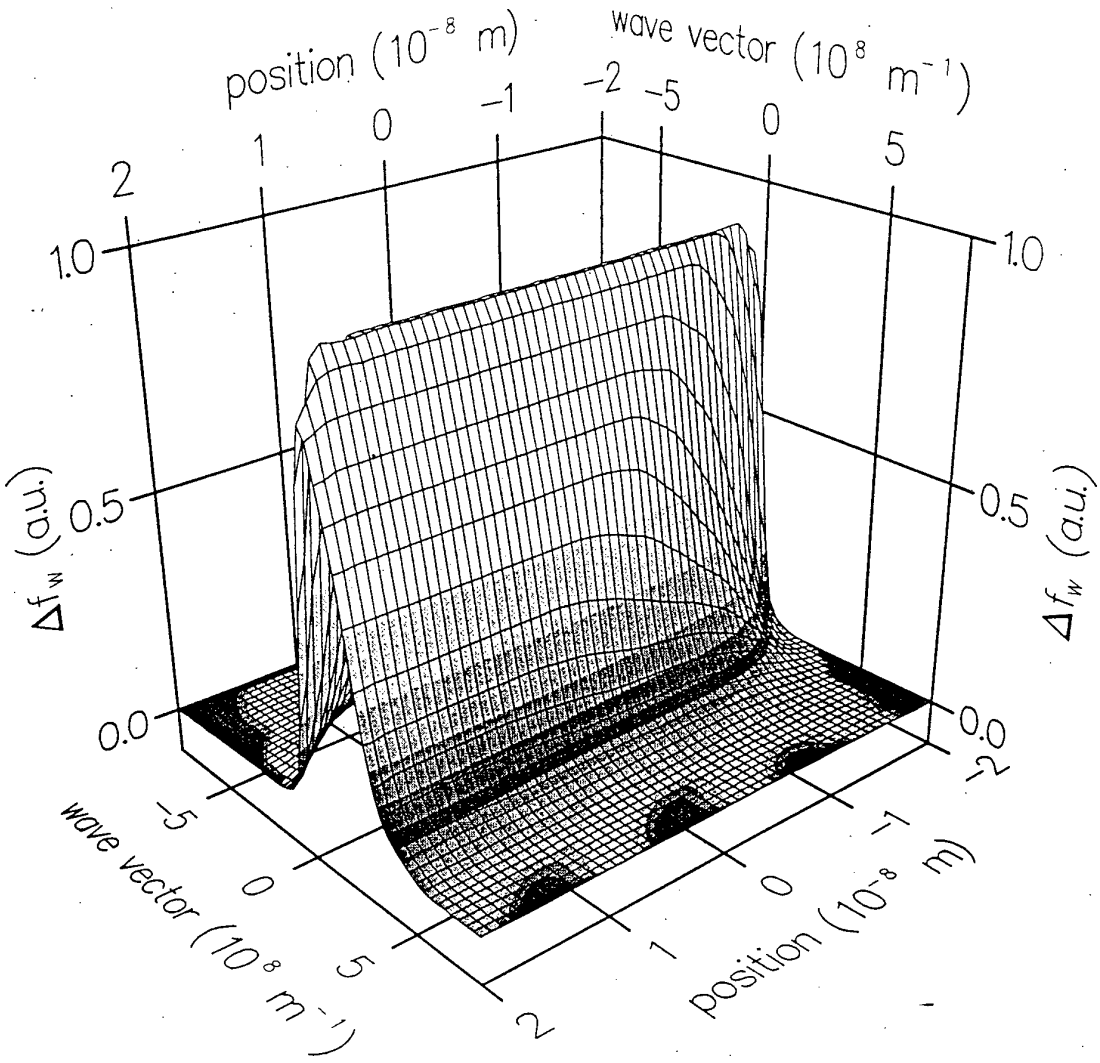
0
5
2
1
0
-1
-2
position (10⁻⁸ m)

Fig 4


position (10^{-8} m)
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1
0
−1
−2
wave vector (10^{8} m^{-1})
−5
0
5
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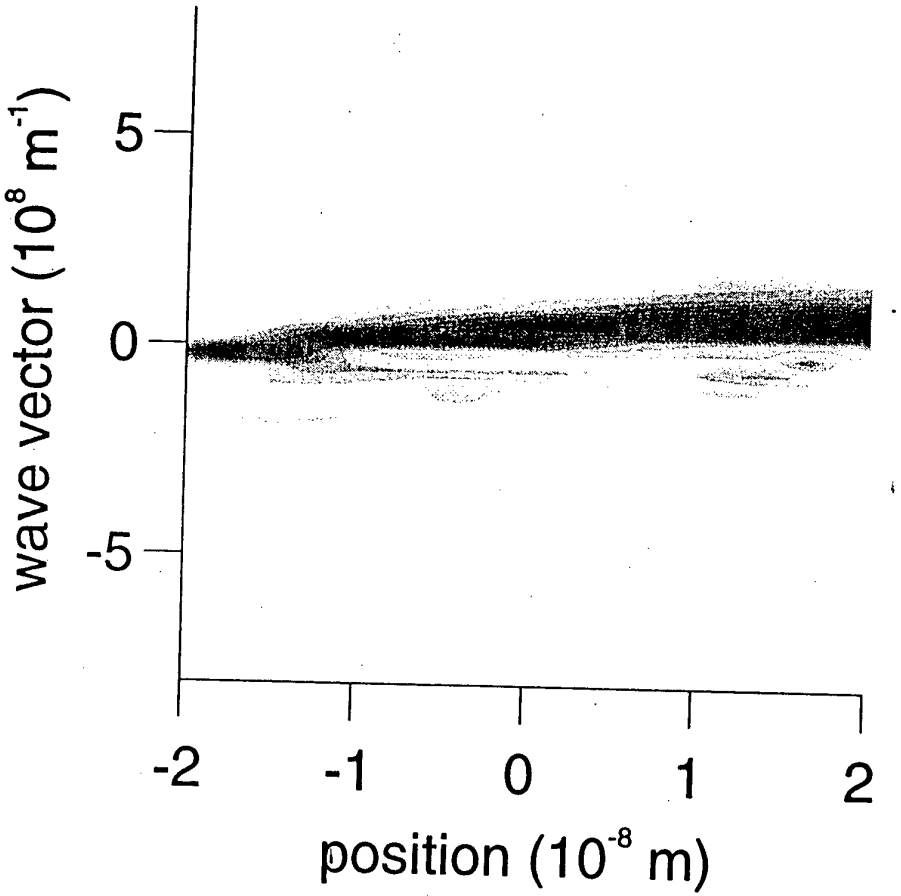
0.5
0.0
Δf_w (a.u.)
wave vector (10^{8} m^{-1})
position (10^{-8} m)

Fig. 5



9.844
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