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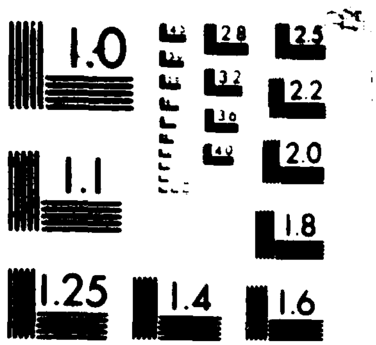

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Frequency-Dependent v-Representability in Density Functional Theory

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University of California, Santa Barbara

Santa Barbara, CA 93106

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Frequency-Dependent v-Representability in Density Functional Theory

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ABSTRACT: In density functional theory (DFT) of the ground state a density distribution, $n_o(\mathbf{r})$, is called v-representable (VR) if it is the ground state density in some external potential. (It is known that not all "reasonable" $n_o(\mathbf{r})$ are VR.) In DFT of time-dependent linear response of a non-degenerate ground state a similar question arises: Is a response density, $n_1(\mathbf{r};\omega)e^{-i\omega t}$, VR; *i.e.*, is it the response to *some* perturbing potential $v_1(\mathbf{r},\omega)e^{-i\omega t}$? (E.K.U. Gross and W. Kohn, Phys. Rev. Lett. 55, 2850 (1985).) In the present paper we show that (1), if the frequency $\omega < \omega_{min}$ (the lowest excitation frequency), the answer is affirmative; and (2), if $\omega > \omega_{min}$, the answer is not necessarily affirmative, as demonstrated by counterexamples. (We exhibit "reasonable" functions $n_1(\mathbf{r},\omega)e^{-i\omega t}$ which, at isolated frequencies, are not VR.) Implications for time-dependent DFT of linear response are discussed.

I. INTRODUCTION

The question under what conditions a static density distribution, $n_o(\mathbf{r})$, is v-representable (VR)[1] has attracted interest in recent years.[2,3,4] The issue of v-representability also arises for time-dependent densities, $n(\mathbf{r},t)$. In particular, in connection with time-dependent linear response[5] one encounters the following situation: Let Ψ_o be the non-degenerate ground state of a many electron system with density $n_o(\mathbf{r})$, in a static external potential $v_o(\mathbf{r})$. A small perturbing potential, $v_1(\mathbf{r},\omega)e^{-i\omega t}$, is known to lead to a unique first order density response, $n_1(\mathbf{r},\omega)e^{-i\omega t}$, where n_1 and v_1 are related by the response function χ:

$$n_1(\mathbf{r},\omega) = \int \chi(\mathbf{r},\mathbf{r}';\omega)v_1(\mathbf{r}',\omega)d\mathbf{r}'. \tag{1}$$

The converse question is, can a given function, $n_1(\mathbf{r},\omega)$, be generated by some function $v_1(\mathbf{r},\omega)$? This is the v-representability problem of linear density response theory addressed in this paper. It may be posed for interacting as well as non-interacting particles.

II. NON-INTERACTING FERMIONS

For non-interacting fermions, first order time-dependent perturbation theory gives the following result for the response function:

$$\chi_s(\mathbf{r},\mathbf{r}';\omega) = \sum_{i,j}(f_i - f_j)\,\frac{\phi_i^*(\mathbf{r})\phi_j(\mathbf{r})\phi_j^*(\mathbf{r}')\phi_i(\mathbf{r}')}{\omega - (\epsilon_j - \epsilon_i) + i\delta}, \tag{2}$$

where ϕ_i are the single particle eigenfunctions of the unperturbed hamiltonian, ϵ_i the eigenvalues, f_i the occupation numbers (1 or 0) for the ground state, and δ is a positive infinitesimal.

Except at the resonances, $\omega = \epsilon_j - \epsilon_i$, χ_s is hermitian and real and has a complete set of orthonormal eigenfunctions, $\varsigma_\ell(\mathbf{r},\omega)$, and real eigenvalues, $\lambda_\ell(\omega)$:

$$\int \chi_s(\mathbf{r},\mathbf{r}';\omega)\varsigma_\ell(\mathbf{r}',\omega)d\mathbf{r}' = \lambda_\ell(\omega)\varsigma_\ell(\mathbf{r},\omega). \tag{3}$$

If, for some frequency $\bar{\omega}$, one of the eigenvalues, say $\lambda_{\bar{\ell}}$, vanishes then the perturbing potential

$$\bar{v}_1(\mathbf{r},\bar{\omega}) \equiv \mu\varsigma_{\bar{\ell}}(\mathbf{r},\bar{\omega}) \tag{4}$$

($\mu << 1$) has vanishing first order density response:

$$\begin{aligned}\bar{n}_1(\mathbf{r},\bar{\omega}) &= \int \chi_s(\mathbf{r},\mathbf{r}';\bar{\omega})\bar{v}_1(\mathbf{r}',\bar{\omega})d\mathbf{r}' \\ &= \mu\lambda_{\bar{\ell}}(\bar{\omega})\varsigma_{\bar{\ell}}(\mathbf{r},\bar{\omega}) = 0.\end{aligned} \tag{5}$$

Also, clearly, the density change

$$n_1(\mathbf{r},\bar{\omega}) \equiv \mu\varsigma_{\bar{\ell}}(\mathbf{r},\bar{\omega}) \tag{6}$$

is not induced by any linear combination of the complete set $\varsigma_\ell(\mathbf{r},\bar{\omega})$, that is, it is not VR as a linear response density.

Conversely, if all $\lambda_\ell(\omega) \neq 0$ any density that can be expressed by a series of the complete set of eigenfunctions,

$$n_1(\mathbf{r},\omega) = \sum_\ell n_{1,\ell}(\omega)\varsigma_\ell(\mathbf{r},\omega), \tag{7}$$

is VR by the potential

$$v_1(\mathbf{r},\omega) = \sum_\ell \lambda_\ell(\omega) n_{1,\ell}(\omega)\varsigma_\ell(\mathbf{r},\omega), \tag{8}$$

provided that the latter series converges.

For all frequencies there exists one vanishing eigenvalue, corresponding to the trivial perturbation v_1 = const. (The corresponding n_1 = const. is trivially not VR.) We shall show that for any system at frequencies smaller than the first resonance no non-trivial vanishing eigenvalues exist, and hence all densities which have a sufficiently rapidly convergent expansion in the functions ς_ℓ are VR.

Restricting attention to non-resonant frequencies and choosing the eigenfunctions ϕ_i real, Eq. (2) may be written as

$$\chi_s(\mathbf{r},\mathbf{r}';\omega) = \sum_{\alpha,\beta} \frac{2\epsilon_{\beta\alpha}}{\omega^2 - \epsilon_{\beta\alpha}^2} \phi_\alpha(\mathbf{r})\phi_\beta(\mathbf{r})\phi_\beta(\mathbf{r}')\phi_\alpha(\mathbf{r}'), \tag{9}$$

where the indices α and β denote the occupied and unoccupied levels, respectively. The response is

$$n_1(\mathbf{r},\omega) = \sum_{\alpha,\beta} \frac{2\epsilon_{\beta\alpha}}{\omega^2 - \epsilon_{\beta\alpha}^2} V_{\beta\alpha}\phi_\alpha(\mathbf{r})\phi_\beta(\mathbf{r}), \tag{10}$$

where

$$V_{\beta\alpha} \equiv \int \phi_\beta(\mathbf{r}) v_1(\mathbf{r},\omega)\phi_\alpha(\mathbf{r}) d\mathbf{r}. \tag{11}$$

The matrix elements $V_{\beta\alpha}$ cannot all vanish, otherwise the determinantal wavefunction perturbed by v_1 would be identical to the unperturbed ground state. The integral

$$\int n_1(\mathbf{r},\omega) v_1(\mathbf{r},\omega) d\mathbf{r} = \sum_{\alpha,\beta} \frac{2\epsilon_{\beta\alpha}}{\omega^2 - \epsilon_{\beta\alpha}^2} V_{\beta\alpha}^2 \tag{12}$$

is then negative-definite for frequencies below the first resonance. Therefore, n_1 can not vanish identically, and χ_s can have no vanishing eigenvalue in this range.

Let us note in passing that, for the special case of a single particle, the density change is

$$n_1(\mathbf{r},\omega) = \phi_1(\mathbf{r}) \sum_{\beta} \frac{2\epsilon_{\beta 1}}{\omega^2 - \epsilon_{\beta 1}^2} V_{\beta 1}\phi_\beta(\mathbf{r}). \tag{13}$$

Owing to the linear independence of the eigenfunctions, ϕ_β, n_1 can not vanish identically at *any* frequency.

We shall now present two examples of systems which, at isolated frequencies above the first resonance, have non-VR response densities.

A. One-dimensional Ring, $v_o = 0$

For a one-dimensional ring, $0 \leq x \leq 2\pi$, the non-interacting eigenfunctions are plane waves:

$$\phi_\ell(x) = (2\pi)^{-1/2}\, e^{i\,k_\ell x}. \tag{14}$$

In the common gauge, k_ℓ is an integer. The ground state with one particle is of no interest (always VR). The ground state with two particles is two-fold degenerate and hence inadmissable for our purposes. However, by choosing an appropriate constant gauge, the allowed k_ℓ are all shifted by $\frac{1}{2}$ so that $k_\ell = (2\ell+1)/2$, $\ell = 0, \pm 1, \pm 2, \ldots$. In this gauge, the two-particle ground state is non-degenerate. Eq.(2) takes the form

$$\chi_s(x,x';\omega) = \frac{1}{2\pi}\sum_{\alpha,\beta}\left[\frac{e^{i(k_\beta-k_\alpha)x}\; e^{-i(k_\beta-k_\alpha)x'}}{\omega-\epsilon_{\beta\alpha}} - \frac{e^{-i(k_\beta-k_\alpha)x}\; e^{i(k_\beta-k_\alpha)x'}}{\omega+\epsilon_{\beta\alpha}}\right], \tag{15}$$

where

$$\epsilon_{\beta\alpha} = k_\beta^2 - k_\alpha^2. \tag{16}$$

The eigenfunctions of χ_s are plane waves, independent of ω, so that

$$\chi_s = \sum_{\ell \neq 0} \lambda_\ell(\omega) \varsigma_\ell(x) \varsigma_\ell^*(x'), \tag{17}$$

where

$$\varsigma_\ell(x) = (2\pi)^{-1/2}\, e^{i\ell x}, \tag{18}$$

and

$$\begin{aligned} \lambda_\ell(\omega) &= \sum_{\substack{\alpha,\beta \\ (k_\beta - k_\alpha = \ell)}} \frac{1}{\omega - (k_\beta^2 - k_\alpha^2)} - \sum_{\substack{\alpha,\beta \\ (k_\beta - k_\alpha = -\ell)}} \frac{1}{\omega + (k_\beta^2 - k_\alpha^2)} \\ &= \sum_{\substack{\alpha \\ (|k_\alpha + \ell| > k_N)}} \frac{1}{\omega - (\ell^2 + 2\ell k_\alpha)} - \sum_{\substack{\alpha \\ (|k_\alpha - \ell| > k_N)}} \frac{1}{\omega + (\ell^2 - 2\ell k_\alpha)}, \end{aligned} \tag{19}$$

with N the number of particles. For example, for $N = 2$, $k_N = 1$ and $k_\alpha = \pm\frac{1}{2}$ so that

$$\begin{aligned} \lambda_{\pm 1}(\omega) &= \frac{4}{\omega^2 - 4} \\ \lambda_\ell(\omega) &= \frac{2(\ell^2 + \ell)}{\omega^2 - (\ell^2 + \ell)^2} + \frac{2(\ell^2 - \ell)}{\omega^2 - (\ell^2 - \ell)^2};\ |\,\ell\,| > 1. \end{aligned} \tag{20}$$

Hence each λ_ℓ, $|\ell| > 1$, has two poles, with a zero lying between them at $\bar{\omega} = \ell(\ell^2 - 1)^{1/2}$.

B. One-dimensional Box, $v_\circ = 0$

For a one-dimensional box, $0 \leq x \leq \pi$, the non-interacting eigenfunctions are standing waves:

$$\phi_\ell(x) = (2/\pi)^{1/2} \sin \ell x, \tag{21}$$

where $\ell = 1, 2, 3, \ldots$, and so

$$\chi_s(x, x'; \omega) = \frac{4}{\pi} \sum_{\alpha,\beta} \frac{\epsilon_{\beta\alpha}}{\omega^2 - {\epsilon_{\beta\alpha}}^2} \sin\alpha x \sin\beta x \sin\beta x' \sin\alpha x', \tag{22}$$

where

$$\epsilon_{\beta\alpha} = \beta^2 - \alpha^2. \tag{23}$$

With the expansion

$$v_1(x,\omega) = \sum_{\ell=1}^{\infty} a_\ell(\omega)\cos\ell x, \tag{24}$$

the matrix elements, Eq. (11), take the form

$$V_{\beta\alpha} = \frac{1}{2}(a_{\beta-\alpha} - a_{\beta+\alpha}), \tag{25}$$

hence

$$n_1(x,\omega) = \frac{1}{\pi}\sum_{\alpha,\beta} \frac{\epsilon_{\beta\alpha}}{\omega^2 - \epsilon^2_{\beta\alpha}}\,(a_{\beta-\alpha}(\omega) - a_{\beta+\alpha}(\omega))\,[\cos(\beta-\alpha)x - \cos(\beta+\alpha)x]. \tag{26}$$

The eigenvalues and eigenfunctions of χ_s are given by

$$n_1(x,\omega) = \lambda(\omega)v_1(x,\omega). \tag{27}$$

For two particles this leads to the set of equations:

$$\lambda a_1 = \frac{1}{\pi}\,\frac{5}{\omega^2-5^2}\,(a_1 - a_5)$$

$$\lambda a_2 = \frac{1}{\pi}\left\{\frac{8}{\omega^2-8^2}\,(a_2 - a_4) + \frac{12}{\omega^2-12^2}\,(a_2 - a_6)\right\}$$

$$\lambda a_3 = \frac{1}{\pi}\left\{\frac{15}{\omega^2-15^2}\,(a_3 - a_5) + \frac{21}{\omega^2-21^2}\,(a_3 - a_7)\right\}$$

$$\lambda a_4 = \frac{1}{\pi}\left\{\frac{24}{\omega^2-24^2}\,(a_4 - a_6) + \frac{32}{\omega^2-32^2}\,(a_4 - a_8) - \frac{8}{\omega^2-8^2}\,(a_2 - a_4)\right\}$$

$$\lambda a_\ell = \frac{1}{\pi}\left\{\frac{(\ell+1)^2-1}{\omega^2-[(\ell+1)^2-1]^2}\,(a_\ell - a_{\ell+2}) + \frac{(\ell+2)^2-4}{\omega^2-[(\ell+2)^2-4]^2}\,(a_\ell - a_{\ell+4})\right.$$
$$\left. - \frac{(\ell-1)^2-1}{\omega^2-[(\ell-1)^2-1]^2}\,(a_{\ell-2} - a_\ell) - \frac{(\ell-2)^2-4}{\omega^2-[(\ell-2)^2-4]^2}\,(a_{\ell-4} - a_\ell)\right\}; \quad \ell \geq 5. \tag{28}$$

Since the even and odd Fourier components are not coupled the eigenfunctions have definite parity. Numerical solutions of the equations corresponding to even eigenfunctions have been carried out for frequencies $0 \leq \omega \leq 50$. The method consists of taking a finite series for Eq. (24), so that the solution of Eqs. (28) is reduced to diagonalization of a finite matrix. Since for any fixed ω the series of Eq. (22) is uniformly convergent in the variables x and x', χ_s can be approximated with arbitrary accuracy by a sufficiently large matrix, for any fixed frequency range.

A plot of the eigenvalues for a 30-dimensional matrix, Fig. 1, exhibits two eigenvalues passing through zero, above the resonances at 12 and 32. Fig. 2 is an expanded view of the first zero in which the repulsion between the eigenvalues, indicating a mixing between the eigenfunctions in regions of near-degeneracy, is more pronounced. Despite this mixing the eigenfunction corresponding to the vanishing eigenvalue tends to a limit as the eigenvalue approaches zero from above, as shown in Fig. 3 for the first zero. Fig. 4 is a plot of the eigenfunction at a frequency for which the eigenvalue is very small and positive. It is given by a rapidly converging Fourier series and, accordingly, is smooth in appearance.

III. INTERACTING FERMIONS

The response function for N interacting fermions is

$$\chi(\mathbf{r},\mathbf{r}';\omega) = \sum_{k=1}^{\infty} \frac{2E_{ko}}{\omega^2 - E_{ko}^2} \int \Psi_o(\mathbf{r},\mathbf{r}_2,\cdots,\mathbf{r}_N)\Psi_k(\mathbf{r},\mathbf{r}_2,\cdots,\mathbf{r}_N)d\mathbf{r}_2\cdots d\mathbf{r}_N$$

$$\times \int \Psi_k(\mathbf{r}',\mathbf{r}'_2,\cdots,\mathbf{r}'_N)\Psi_o(\mathbf{r}',\mathbf{r}'_2,\cdots,\mathbf{r}'_N)d\mathbf{r}'_2\cdots \mathbf{r}'_N, \quad (29)$$

where E_i and Ψ_i $(0 \leq i < \infty)$ are the eigenvalues and normalized eigenfunctions of the N-particle hamiltonian, and $E_{ko} = E_k - E_o$. The relations analogous to Eqs. (10) and (12) for the non-interacting case are

$$n_1(\mathbf{r},\omega) = \sum_{k=1}^{\infty} \frac{2E_{ko}}{\omega^2 - E_{ko}^2} V_{ko} \int \Psi_o(\mathbf{r},\mathbf{r}_2,\cdots,\mathbf{r}_N)\Psi_k(\mathbf{r},\mathbf{r}_2,\cdots,\mathbf{r}_N)d\mathbf{r}_2\cdots d\mathbf{r}_N \quad (30)$$

and

$$\int n_1(\mathbf{r},\omega)v_1(\mathbf{r},\omega)d\mathbf{r} = \sum_{k=1}^{\infty} \frac{2E_{ko}}{\omega^2 - E_{ko}^2} V_{ko}^2, \quad (31)$$

where

$$V_{ko} \equiv N \int \Psi_k(\mathbf{r}_1,\mathbf{r}_2,\cdots \mathbf{r}_N)v_1(\mathbf{r}_1)\Psi_o(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)d\mathbf{r}_1 d\mathbf{r}_2\cdots d\mathbf{r}_N. \quad (32)$$

Eq. (31), like Eq. (12), is negative-definite for frequencies below the first resonance. Therefore, exactly as shown in Sec. I for χ_s, it follows that χ can have no vanishing eigenvalues in this range.

IV. CONCLUDING REMARKS

In their paper on density functional theory of linear response, Gross and Kohn[5] presupposed that the physical density $n_o(\mathbf{r}) + n_1(\mathbf{r},t)$ was "non-interacting VR" (VR-N), that is, can be reproduced by a system of non-interacting particles in an external potential $v_o(\mathbf{r}) + v_1(\mathbf{r},t)$. We have shown in this paper that this will be the case if n_o by itself is VR-N and the frequency of v_1 is less than the smallest resonance. However, if the frequency is higher, our examples show that caution is in order. If our examples are representative, then in general we expect that there will be *isolated* frequencies, $\bar{\omega}$, at which *most* density changes are *not* VR-N. The exceptions are those special functions which are orthogonal to the functions $\zeta_l(\mathbf{r},\bar{\omega})$, corresponding to vanishing eigenvalues of χ_s.

We note, however, that in the special case of an infinite uniform non-interacting electron gas the response function $\chi(\mathbf{k},\omega)$ has no vanishing eigenvalues for any $\mathbf{k}$ or ω, so that any sufficiently regular $n_1(\mathbf{r},\omega)$ is VR-N at all frequencies.

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FIGURE CAPTIONS

Fig. 1. Eigenvalues of χ_s for a 30-dimensional matrix. The dashed lines mark the locations of the resonances at $\omega = 8$, 12, 24, 32, and 48.

Fig. 2. Eigenvalues of χ_s in a frequency range containing a zero.

Fig. 3. Magnitudes of the first 10 Fourier amplitudes of an eigenfunction with eigenvalue tending to zero, weighted so that $(\pi/2)^{1/2}\sum_\ell |a_\ell|^2 = 1$. The dashed line is the eigenvalue curve in the same frequency range (vertical scale not shown).

Fig. 4. Normalized eigenfunction for $\lambda(\omega) = 1.2386\times10^{-5}$, $\omega = 12.658$.

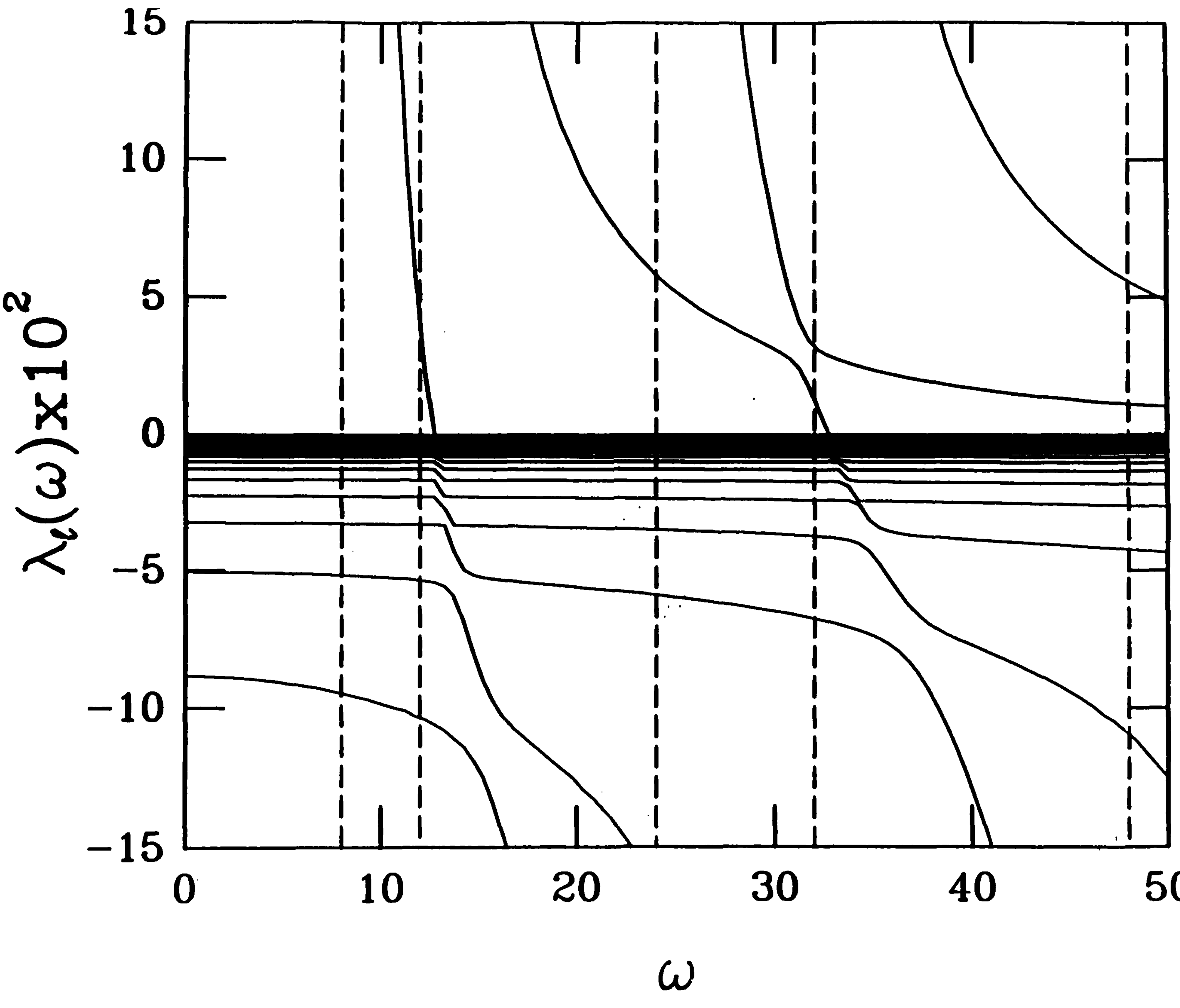

Fig 1

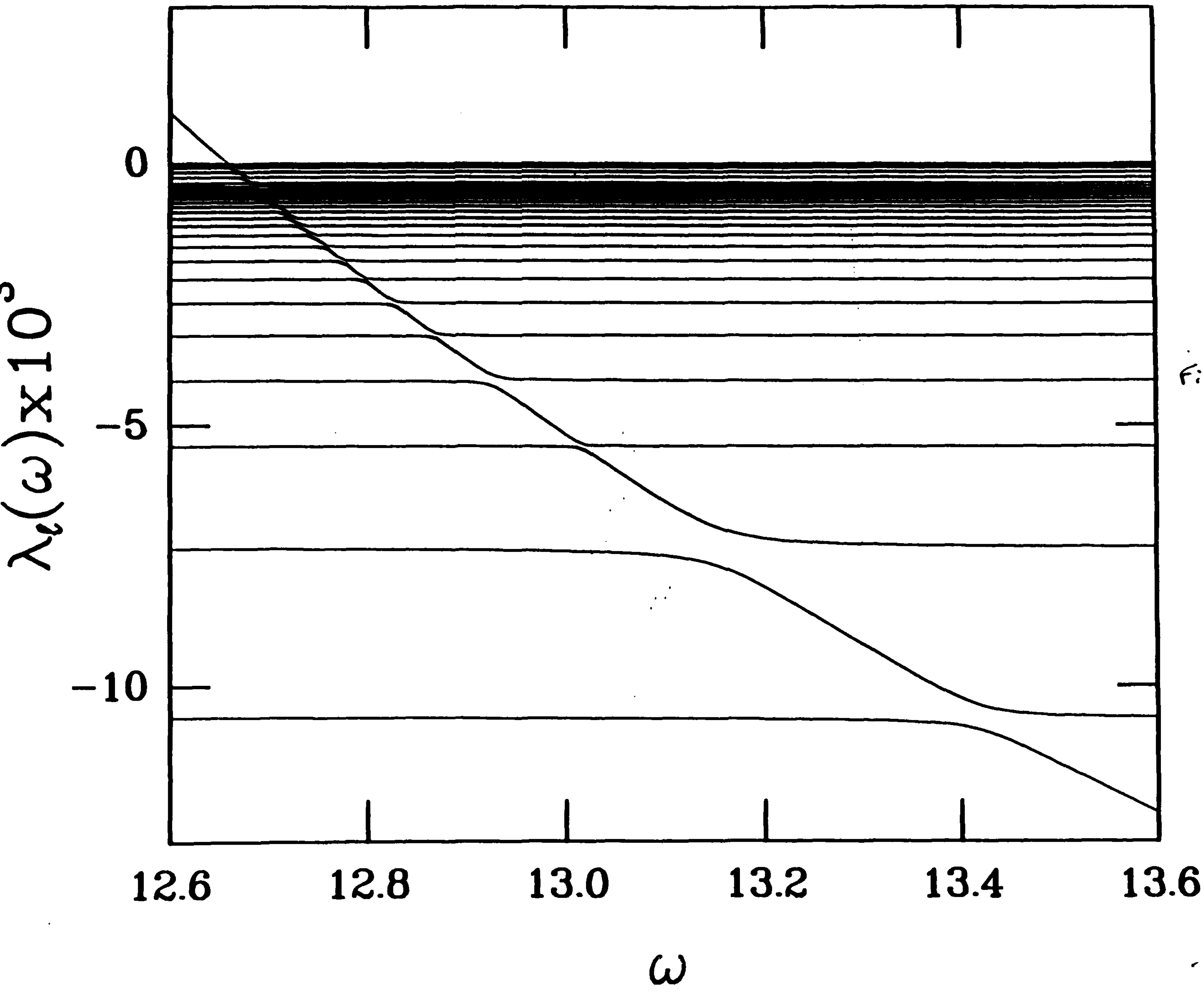

Fig. 2

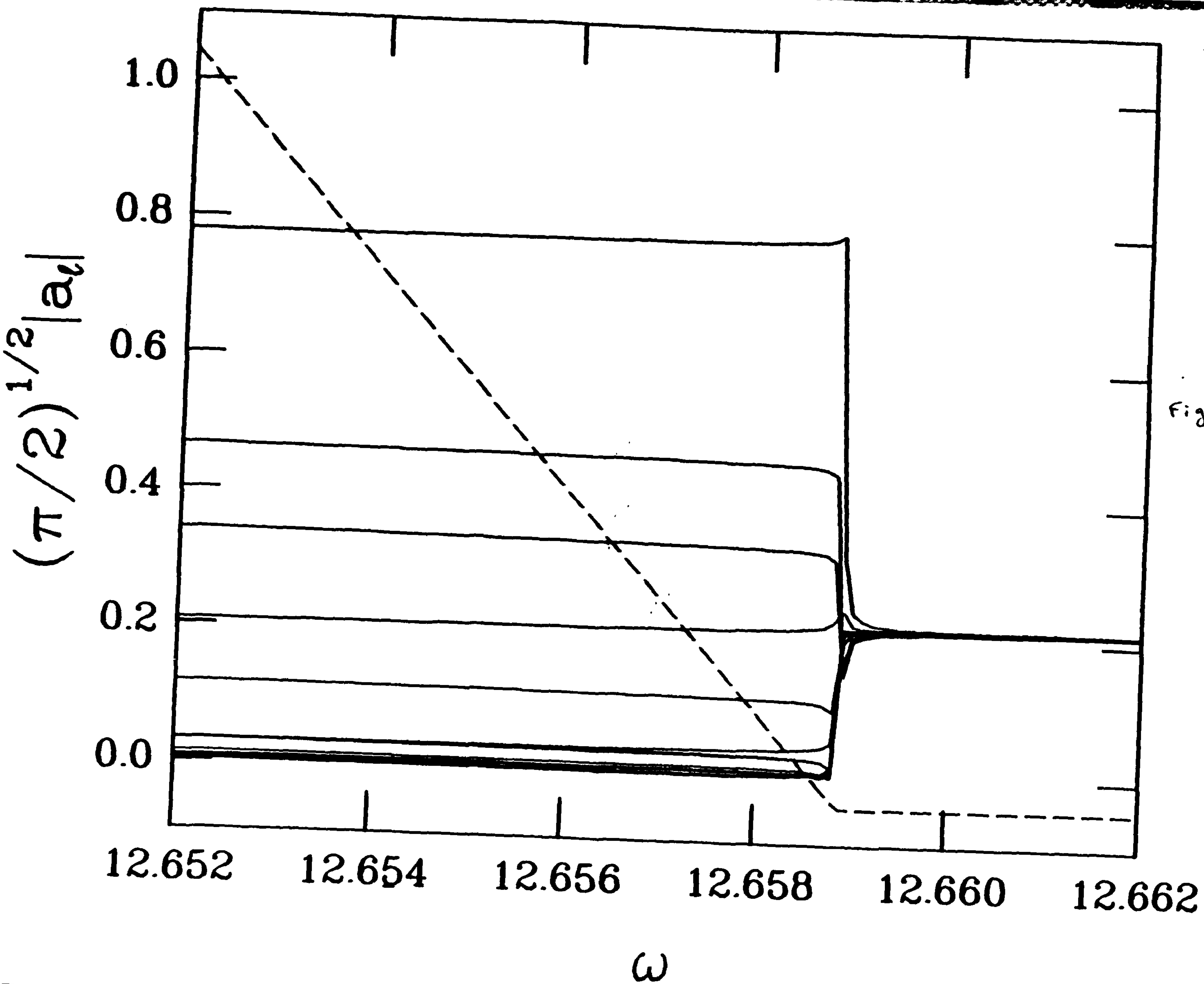
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Fig. 3

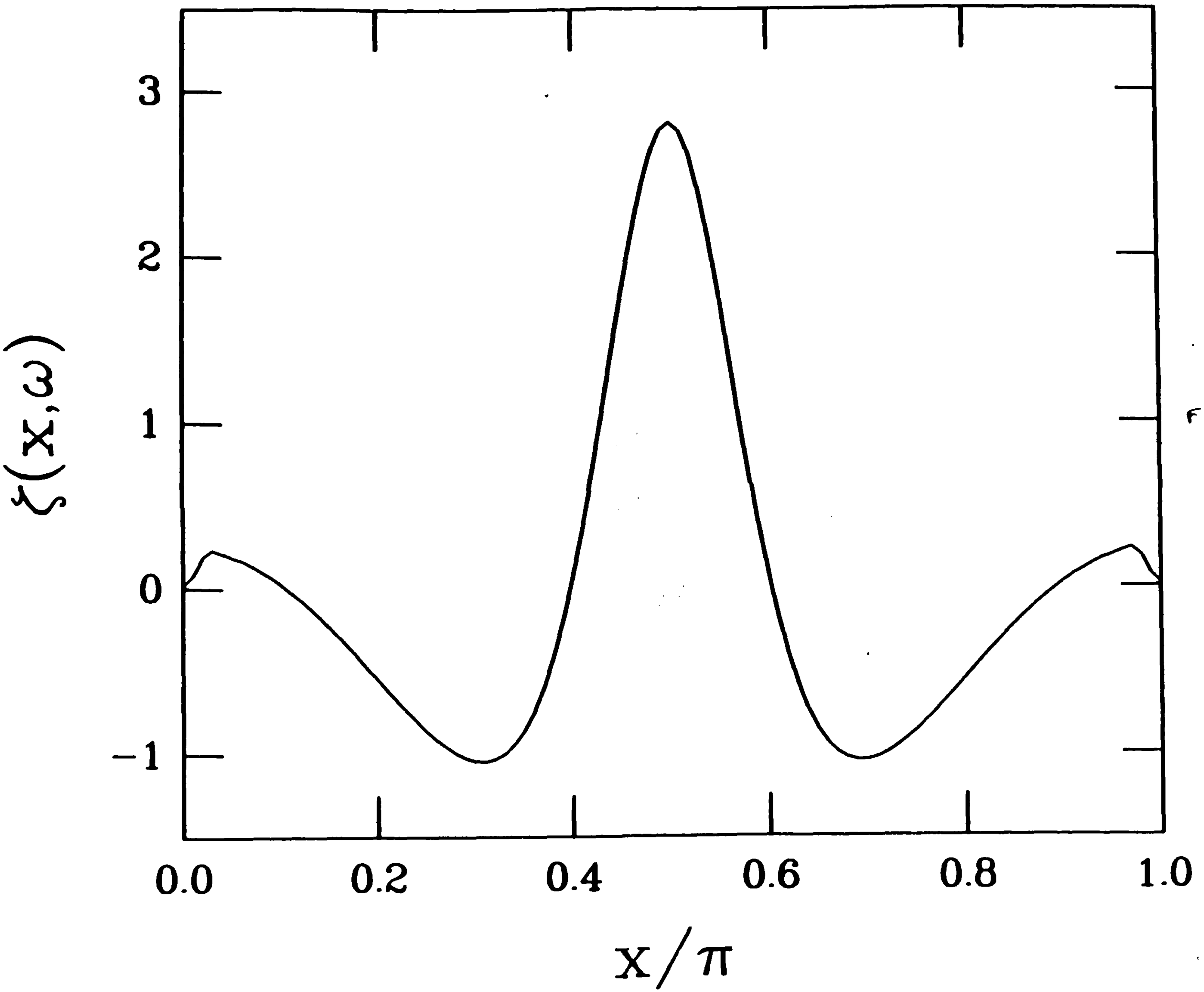

Fig. 4

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