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Nonlinear renormalization of the surface-order-parameter interface Hamiltonian

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Abstract. The coupling between order-parameter fluctuations near the wall and depinning fluid interface in the approach to a complete wetting transition is described by a two-field Hamiltonian $H_2[l_1, l_2]$ which improves upon standard capillary-wave models of wetting. We construct a nonlinear renormalization group to study fluctuation effects in $d = 3$ and show how this elegantly rederives the expression for the renormalized wetting parameter found in earlier (linear) renormalization-group treatments.

At a wetting transition the adsorption of a phase β intruding between bulk phases α and γ changes from a microscopic to macroscopic value [1]. It is common to view this as an example of interfacial unbinding [2]. For example, in a binary liquid mixture the two interfaces (denoted $\alpha|\beta$ and $\beta|\gamma$, respectively) are both fluid and hence rough in the limit of infinite separation for $d \leqslant 3$ (see figure 1(a)). For a one component fluid on the other hand, adsorption at a planar wall is often modelled as the interaction of a single fluid $\alpha|\beta$ interface with a rigid $\beta|\gamma$ surface which has no fluctuations (figure 1(b)). However, recent work [3–5] on the structure of correlation functions at the complete wetting transition has shown that the latter interpretation neglects important coupling effects between order-parameter fluctuations at the wall and $\alpha|\beta$ interface which may be modelled using a novel two-field Hamiltonian $H_2[l_1, l_2]$. This approach successfully describes qualitative and quantitative features of correlation function behaviour [6–8] which are inexplicable using the standard interfacial model. In this paper we study the renormalization of $H_2[l_1, l_2]$ using a straightforward generalization of the nonlinear renormalization group (RG) scheme of Lipowsky and Fisher [9, 10] (see also the review [2]) and show how this elegantly rederives the linear RG expression [11] for the renormalized wetting (or capillary) parameter $\bar{\omega}$ determining values of critical amplitudes for complete wetting with short-ranged forces in $d = 3$.

To begin we briefly recall how the wetting parameter enters the binding potential flow equation in linear and nonlinear RG treatments of standard effective Hamiltonian models [12]. For wetting by a simple fluid at a planar wall this has the form [1, 2]

$$H_I[l(\boldsymbol{y})] = \int \mathrm{d}\boldsymbol{y} \left\{ \tfrac{1}{2} \Sigma_{\alpha\beta} (\nabla l(\boldsymbol{y}))^2 + W(l(\boldsymbol{y})) \right\} \tag{1}$$

where $\Sigma_{\alpha\beta}$ is the stiffness coefficient of the free liquid–vapour interface that unbinds from the wall and $W(l)$ is the binding potential. The collective coordinate $l(\boldsymbol{y})$ is a measure of

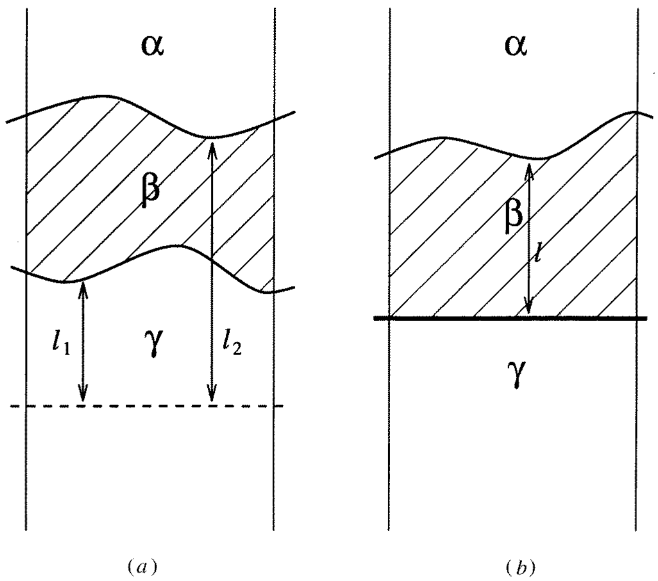

Figure 1. Two geometries in which an adsorbed phase β intrudes between the bulk phases α and γ. In (a) a binary liquid mixture is shown with two fluctuating interfaces—the variables l_1 and l_2 denote the local distance of the two fluid–fluid interfaces from some reference plane. In (b) a layer of phase β is adsorbed between the solid substrate (γ) and phase α. Here l denotes the position of the $\alpha|\beta$ interface.

the thickness of the adsorbed layer at vector displacement $\boldsymbol{y}$ along the wall. For wetting in a binary liquid mixture one similarly writes

$$H_I[l_1, l_2] = \int \mathrm{d}\boldsymbol{y}\{\tfrac{1}{2}\Sigma_{\beta\gamma}(\nabla l_1)^2 + \tfrac{1}{2}\Sigma_{\alpha\beta}(\nabla l_2)^2 + W(l_2 - l_1)\} \tag{2}$$

which clearly allows for fluctuations of both interfaces (the positions of which are described by a pair of collective coordinates $l_1(\boldsymbol{y})$ and $l_2(\boldsymbol{y})$). In fact the binary Hamiltonian (2) can be decoupled and the relative interaction transformed into the single interface form (1) by introducing relative ($l_{21} = l_2 - l_1$) and 'centre-of-mass' coordinates [2]. The effective stiffness $\bar{\Sigma}$ satisfies the relation [13]

$$\frac{1}{\bar{\Sigma}} = \frac{1}{\Sigma_{\alpha\beta}} + \frac{1}{\Sigma_{\beta\gamma}}\,. \tag{3}$$

This expression appears as a limiting case in RG treatments of the two-field Hamiltonian describing complete wetting by a simple fluid [3, 11] which will be discussed below.

Before considering the two-field Hamiltonian model we recapitulate the linear and nonlinear RG treatments of the single interface model (1). Generally the initial (bare) binding potential $W^{(0)}(l) \equiv W(l)$ is renormalized according to

$$W^{(1)}(l) = \mathcal{R}[W^{(0)}(l)] \tag{4}$$

where $\mathcal{R}$ is the appropriate recursion operator. Note that implicit in the Hamiltonian definitions (1) and (2) is a momentum cut-off Λ (or equivalently a short-distance cut-off Λ^{-1}). The RG procedure involves dividing the fluctuating field $l(\boldsymbol{y})$ into long-wavelength ($l^<(\boldsymbol{y})$) and short-wavelength ($l^>(\boldsymbol{y})$) parts, where $l^<$ and $l^>$ contain all Fourier components of l with wavenumbers $|\boldsymbol{k}| < \Lambda/b$ and $\Lambda/b < |\boldsymbol{k}| < \Lambda$, respectively. Here $b > 1$ is the usual arbitrary spatial rescaling factor. The recursion operator is determined by integrating out the short-wavelength fluctuations via some approximation and rescaling in order to bring the momentum cut-off back to its original value.

Within the simplest (linear) RG scheme the trace over $l^>$ is simplified by expanding the binding potential about $l^<$ and working only to first order in $W(l)$. In $d = 3$ this procedure yields [12]

$$\mathcal{R}[W(l)] = b^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}l'}{\sqrt{2\pi}\,\tilde{a}(b)} W(l') \exp\left\{-\frac{(l-l')^2}{2\tilde{a}^2(b)}\right\} \tag{5}$$

where

$$\tilde{a}^2(b) = \frac{k_B T}{2\pi\,\Sigma_{\alpha\beta}} \ln b\,. \tag{6}$$

In the infinitesimal rescaling limit $b = e^{\delta t}\,(\delta t \to 0)$ the recursion relation (5) leads to the simple flow equation

$$\frac{\mathrm{d}W}{\mathrm{d}t} = 2W + \omega \frac{\partial^2 W}{\partial l^2} \tag{7}$$

where ω is the dimensionless wetting parameter defined as

$$\omega = \frac{k_B T}{4\pi\,\Sigma_{\alpha\beta}\xi_b^2}\,. \tag{8}$$

In this analysis, and those described below, distances in the l direction have been measured in terms of the bulk correlation length ξ_b of the wetting phase (which henceforth we set to unity without loss of generality). The value of the wetting parameter determines non-universal critical amplitudes at complete wetting in three-dimensional systems with short-ranged forces [12] corresponding to the marginal dimensionality [13].

A nonlinear RG treatment of (1) has been performed by Lipowsky and Fisher [9, 10] who consider an extension of Wilson's original scheme [14]. This method necessarily leads to the vanishing of the critical point decay exponent η—however, for wetting transitions $\eta = 0$ identically [10] and thus the resultant recursion relations are believed to be more reliable for the study of interfacial transitions than for standard bulk critical phenomena. In $d = 3$ this nonlinear treatment yields the recursion relation

$$\mathcal{R}[W(l)] = -\tilde{\nu}(b) b^2 \ln\Bigg[\int_{-\infty}^{\infty} \frac{\mathrm{d}l'}{\sqrt{2\pi}\,\tilde{a}(b)} \times \exp\left\{-\frac{1}{2}\left(\frac{l'}{\tilde{a}(b)}\right)^2 - \frac{1}{2\tilde{\nu}(b)}[W(l-l') + W(l+l')]\right\}\Bigg] \tag{9}$$

where

$$\tilde{\nu}(b) = \frac{k_B T \Lambda^2}{4\pi}\left(1 - \frac{1}{b^2}\right) \tag{10}$$

and $\tilde{a}(b)$ is given by (6). The value of $\tilde{a}(b)$ within this RG scheme is in fact arbitrary but is chosen such that the linear RG result (5) is recovered upon expanding to first order in W. The corresponding flow equation is once again derived by considering the infinitesimal rescaling limit, thus

$$\frac{\mathrm{d}W}{\mathrm{d}t} = 2W + \frac{k_B T \Lambda^2}{4\pi} \ln\left[1 + \frac{4\pi\omega}{k_B T \Lambda^2} \frac{\partial^2 W}{\partial l^2}\right] \tag{11}$$

which clearly rederives (7) to linear order. Hence (11) reveals how the wetting parameter ω enters the nonlinear RG analysis of wetting. Further, a numerical study based upon this analysis [10] reveals that a shift in the origin (i.e. the position of the wall) is a marginal operator in $d = 3$. This provides an early indication that 'non-critical' wall effects may play an important role in unbinding transitions.

We next turn our attention to recent studies which show that in order to derive the correlation function structure at a complete wetting transition in a thermodynamically consistent manner we must allow for coupling between order-parameter fluctuations near the wall and depinning fluid interface [3–5]. This coupling is modelled via a two-field Hamiltonian $H_2[l_1, l_2]$; for the calculation of critical effects described below it is sufficient to write

$$H_2[l_1, l_2] = \int d\boldsymbol{y} \left\{ \tfrac{1}{2}\Sigma_{w\beta}(\nabla l_1)^2 + \tfrac{1}{2}\Sigma_{\alpha\beta}(\nabla l_2)^2 + W(l_1, l_2) \right\}. \tag{12}$$

Here the collective coordinate l_2 represents the position of the unbinding $\alpha|\beta$ interface while l_1 models fluctuations of a non-critical $w\beta$ interface (with associated finite correlation length $\xi_{w\beta}$) which remains bound to the wall in the limit of complete wetting (see [3, 4] for a precise definition). Here $\Sigma_{w\beta}$ represents the stiffness of this non-critical wall-β phase interface. The binding potential $W(l_1, l_2)$ may be separated and written in the form

$$W(l_1, l_2) = U(l_1) + W_{(2)}(l_2 - l_1) \tag{13}$$

where $W_{(2)}$ is the binding potential appropriate for the unbinding of the upper interface from the lower one and is rather similar to $W(l)$ contained in the single-field theory. The term $U(l_1)$ models the fluctuations of the lower interface—these are assumed small and hence $U(l_1)$ may be approximated by expanding around its minimum value l_0 which we set to zero without loss of generality. Thus we write $U(l_1) = rl_1^2/2$. The choice of this Gaussian form has allowed the introduction of a novel RG scheme which involves an exact treatment of the lower surface while treating the relative binding potential $W_{(2)}$ in a purely linear RG fashion [3, 11]. This analysis reveals that $W_{(2)}$ renormalizes in exactly the same manner as $W(l)$ in the single-field theory but with the wetting parameter ω (given by (8)) being replaced by the renormalized quantity

$$\bar{\omega} = \omega + \frac{\omega_\beta}{1 + (\Lambda\xi_{w\beta})^{-2}} \tag{14}$$

where $\omega_\beta = k_B T/4\pi\Sigma_{w\beta}\xi_b^2$ and $\xi_{w\beta}^{-2} = r/\Sigma_{w\beta}$. The renormalization of the wetting parameter as given by (14) is crucial in understanding recent Ising model simulation studies of wetting [15, 16] which, as detailed at length in [11], are inexplicable using a standard effective interfacial Hamiltonian model. We observe that $\bar{\omega}$ displays two limiting behaviours depending on the value of $\xi_{w\beta}$. First, in the limit $\xi_{w\beta} \to 0$ (or $r \to \infty$) the fluctuations of the bound l_1 surface are completely suppressed and we recover the single-field result $\bar{\omega} \equiv \omega$. In the other limit $\xi_{w\beta} \to \infty$ the Hamiltonian $H_2[l_1, l_2]$ reduces to that pertinent to a binary liquid mixture as given in (2). As mentioned earlier the wetting transition in this case is controlled by the effective stiffness $\bar{\Sigma}$ (see equation (3)) which clearly corresponds to the $\xi_{w\beta} = \infty$ result $\bar{\omega} = \omega + \omega_\beta$ which may be read off from (14). As mentioned earlier the renormalization of the wetting parameter within the two-field theory is related to the existence of a marginal operator in the standard capillary-wave model, which translates the origin of the binding potential.

Given that this conclusion is rather surprising we wish to test the robustness of this RG scheme, and hence of the ω renormalization, by considering a nonlinear RG analysis of (12). In particular, we wish to derive the recursion relation and flow equation for the full binding potential $W(l_1, l_2)$ and then confirm the results given above by substituting for $W(l_1, l_2)$ from (13) with $U(l_1) = rl_1^2/2$. The RG procedure commences by dividing both fluctuating fields l_1 and l_2 into long- and short-wavelength parts as discussed above. The short-wavelength components are then expanded in terms of a complete set of suitably chosen eigenfunctions which are assumed localized in both real and momentum space [14]. The intermediate renormalized, unrescaled Hamiltonian $H'[l_1^<, l_2^<]$ is defined via the partial trace over short-wavelength fluctuations

$$\exp\{-\beta H'[l_1^<, l_2^<]\} = \exp\{-\beta H_0[l_1^<, l_2^<]\} \times \frac{\int\int \mathcal{D}l_1^> \mathcal{D}l_2^> \exp\{-\beta(H_0[l_1^>, l_2^>] + H_W[l_1^< + l_1^>, l_2^< + l_2^>])\}}{\int\int \mathcal{D}l_1^> \mathcal{D}l_2^> \exp\{-\beta H_0[l_1^>, l_2^>]\}} \tag{15}$$

where $\beta = 1/k_B T$ and

$$\begin{aligned} H_0[l_1, l_2] &= \int \mathrm{d}\boldsymbol{y} \left\{ \tfrac{1}{2}\Sigma_{w\beta}(\nabla l_1)^2 + \tfrac{1}{2}\Sigma_{\alpha\beta}(\nabla l_2)^2 \right\} \\ H_W[l_1, l_2] &= \int \mathrm{d}\boldsymbol{y}\, W(l_1, l_2) \end{aligned} \tag{16}$$

so that $H_2[l_1, l_2] = H_0[l_1, l_2] + H_W[l_1, l_2]$.

The trace in (15) can be performed by making the same bold approximations as Wilson in his original RG treatment—these are explained particularly clearly in [17]. In order to complete the RG transformation we must rescale the coordinate $\boldsymbol{y}$ according to $\boldsymbol{y} \to \boldsymbol{y}' = \boldsymbol{y}/b$ so that the momentum cut-off is restored to its original value. As a result of this procedure we derive the recursion relation

$$\mathcal{R}[W(l_1, l_2)] = -\tilde{\nu}(b)b^2 \ln\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\mathrm{d}l_1'\,\mathrm{d}l_2'}{2\pi\tilde{a}_1(b)\tilde{a}_2(b)} \exp\left\{-\frac{1}{2}\left(\frac{l_1'}{\tilde{a}_1(b)}\right)^2 - \frac{1}{2}\left(\frac{l_2'}{\tilde{a}_2(b)}\right)^2 - \frac{1}{2\tilde{\nu}(b)}[W(l_1 + l_1', l_2 + l_2') + W(l_1 - l_1', l_2 - l_2')]\right\}\right] \tag{17}$$

where $\tilde{\nu}(b)$ is given by (10) and

$$\tilde{a}_1^2(b) = \frac{k_B T}{2\pi\Sigma_{w\beta}} \ln b \qquad \tilde{a}_2^2(b) = \tilde{a}^2(b) = \frac{k_B T}{2\pi\Sigma_{\alpha\beta}} \ln b \tag{18}$$

are defined in order to correctly recover straightforward linear RG results (i.e. when the full binding potential $W(l_1, l_2)$ is treated in a linear fashion). Exactly as with the earlier analyses we can derive the flow equation for W by considering the infinitesimal rescaling limit $b = e^{\delta t}$ $(\delta t \to 0)$. The resulting equation is

$$\frac{\mathrm{d}W}{\mathrm{d}t} = 2W + \frac{k_B T\Lambda^2}{4\pi} \ln\left[1 + \frac{4\pi\omega_\beta}{k_B T\Lambda^2}\frac{\partial^2 W}{\partial l_1^2} + \frac{4\pi\omega}{k_B T\Lambda^2}\frac{\partial^2 W}{\partial l_2^2} + \frac{16\pi^2\omega\omega_\beta}{(k_B T\Lambda^2)^2}\left(\frac{\partial^2 W}{\partial l_1^2}\frac{\partial^2 W}{\partial l_2^2} - \left\{\frac{\partial^2 W}{\partial l_1 \partial l_2}\right\}^2\right)\right]. \tag{19}$$

By construction, (19) correctly rederives the standard linear RG result on expanding to first order in W. In addition we observe that if W is just a function of the unbinding coordinate l_2 this flow equation reduces exactly to the single-field nonlinear RG result (11).

In order to verify the validity of the quasi-linear RG scheme proposed in [3] we substitute $W(l_1, l_1) = rl_1^2/2 + W_{(2)}(l_2 - l_1)$ into (17) and examine how $W_{(2)}$ renormalizes. The renormalization of the Gaussian term in l_1 is well understood and hence this is easily extracted. The remaining term yields the renormalization of the relative binding potential.

Transforming to relative coordinates allows one of the integrations to be performed and we thus derive

$$\mathcal{R}[W_{(2)}(\Delta l)] = -\tilde{\nu}(b)b^2 \ln\Bigg[\int_{-\infty}^{\infty} \frac{\mathrm{d}\Delta l'}{\sqrt{2\pi}\tilde{\alpha}(b)} \exp\Bigg\{-\frac{1}{2}\left(1+\frac{\tilde{a}_1^2(b)r}{\tilde{\nu}(b)}\right)\left(\frac{\Delta l'}{\tilde{\alpha}(b)}\right)^2 - \frac{1}{2\tilde{\nu}(b)}[W_{(2)}(\Delta l+\Delta l') + W_{(2)}(\Delta l - \Delta l')]\Bigg\}\Bigg] \tag{20}$$

where $\Delta l = l_2 - l_1$ and

$$\tilde{\alpha}^2(b) = \tilde{a}_1^2(b) + \tilde{a}_2^2(b) + \frac{\tilde{a}_1^2(b)\tilde{a}_2^2(b)r}{\tilde{\nu}}\,. \tag{21}$$

Thus, up to constant factors, the flow equation for $W_{(2)}$ is simply

$$\frac{\mathrm{d}W_{(2)}}{\mathrm{d}t} = 2W_{(2)} + \frac{k_B T\Lambda^2}{4\pi}\ln\left[1+\frac{4\pi}{k_B T\Lambda^2}\left\{\omega+\frac{\omega_\beta}{1+(\Lambda\xi_{w\beta})^{-2}}\right\}\frac{\partial^2 W_{(2)}}{\partial\Delta l^2}\right]. \tag{22}$$

Hence comparing with (11) we immediately observe that the ω renormalization is confirmed by this nonlinear RG analysis. Consequently we conclude that this important fluctuation effect related to the coupling of surface fluctuations to those in the unbinding $\alpha|\beta$ interface is robust under a full nonlinear RG analysis.

To conclude we make some closing remarks:

(i) The nonlinear RG analysis presented above demonstrates that the renormalization $\omega \to \bar{\omega}$ is an authentic effect. That is, the renormalization is confirmed not just at first order in $W_{(2)}$ but comparison of (22) and (11) reveals that this effect is true to all orders. It is important to note that although the free parameters $\tilde{a}_1$, $\tilde{a}_2$ are chosen to guarantee that the nonlinear recursion relation (17) recovers the fully linearized two-field recursion formula (which also treats the $rl_1^2/2$ term in linear fashion) they are not chosen to identically rederive the RG flow equation for $W_{(2)}$. Thus we believe that the derived nonlinear flow equation (22) provides an independent confirmation of the so-called wetting parameter renormalization effect.

(ii) In the above discussion we have not considered the inclusion of position dependence in the stiffness coefficients as has recently been suggested for the single-field model [18]. Such position dependence it has been shown to be crucial in the two-field model for understanding next-to-leading order singular behaviour in correlation function structure at wetting transitions [3, 4]. Unfortunately it is not possible to incorporate position-dependent stiffnesses into the nonlinear RG approximations in a consistent manner—at least not within Wilson's original scheme. However, even within the linear RG such terms make no leading-order contribution to critical effects (embodied in the ω renormalization) and hence we are confident that it is safe to ignore them within the present analysis.

(iii) Our above study is restricted to a model of complete wetting away from the critical wetting transition. The two-field theory of critical wetting is somewhat more complicated still because it simultaneously involves the decoupling of modes in the two collective coordinates [5]. The RG analysis [19] predicts that for this transition there is no renormalization of the wetting parameter but does reveal subtle differences from the capillary-wave (see [12] and references therein) and Fisher–Jin [18] theories related to scaling violations which would appear to explain long-standing anomalous Ising model simulation results [20].

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References

[1] For reviews of wetting see for example (a) Schick M 1990 *Les Houches, Session XLVIII: Liquids at Interfaces* ed J Charvolin, J F Joanny and J Zinn-Justin (Amsterdam: North Holland) and (b) Dietrich S 1988 *Phase Transitions and Critical Phenomena* vol 12 ed C Domb and J L Lebowitz (London: Academic).

[2] See for example the review article by Forgács G, Lipowsky R and Nieuwenhuizen Th M 1991 *Phase Transitions and Critical Phenomena* vol 14 ed C Domb and J L Lebowitz (New York: Academic) and also Lipowsky R 1988 *Habilitations-Schrift* Institut für Festköperforschung, Julich.

[3] Boulter C J and Parry A O 1995 *Phys. Rev. Lett.* **74** 3403

[4] Parry A O and Boulter C J 1995 *Physica* **218A** 77

[5] Parry A O and Boulter C J 1996 *Mol. Phys.* to appear

[6] Parry A O and Evans R 1988 *Mol. Phys.* **65** 455

[7] Parry A O and Evans R 1993 *Mol. Phys.* **78** 1527

[8] Parry A O and Boulter C J 1994 *J. Phys.* A **27** 1877

[9] Lipowsky R and Fisher M E 1986 *Phys. Rev. Lett.* **57** 2411

[10] Lipowsky R and Fisher M E 1987 *Phys. Rev.* B **36** 2126

[11] Boulter C J and Parry A O 1995 *Physica* **218A** 109

[12] Fisher D S and Huse D A 1985 *Phys. Rev.* B **32** 247

[13] Lipowsky R 1985 *Phys. Rev.* B **32** 1731

[14] Wilson K G 1971 *Phys. Rev.* B **4** 3184
Wilson K G and Fisher M E 1972 *Phys. Rev. Lett.* **28** 240

[15] Binder K, Landau D P and Ferrenberg A M 1995 *Phys. Rev. Lett.* **74** 298

[16] Binder K, Landau D P and Ferrenberg A M 1995 *Phys. Rev.* E **51** 2823

[17] Ma S-K 1976 *Modern Theory of Critical Phenomena* (New York: Benjamin)

[18] Fisher M E and Jin A J 1992 *Phys. Rev. Lett.* **69** 792

[19] Parry A O and Boulder C J *Preprint*

[20] Binder K, Landau D P and Kroll D M 1986 *Phys. Rev. Lett.* **56** 2272