Home Search Collections Journals About Contact us My IOPscience

Return to coherence via Debye-Waller factor quenching

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 2009 J. Phys.: Condens. Matter 21 405004 (http://iopscience.iop.org/0953-8984/21/40/405004) View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 129.252.86.83 The article was downloaded on 30/05/2010 at 05:31

Please note that terms and conditions apply.

J. Phys.: Condens. Matter 21 (2009) 405004 (6pp)

# **Return to coherence via Debye–Waller** factor quenching

## Andrea C Levi

Dipartimento di Fisica, CNISM and Università di Genova, Via Dodecaneso 33, I-16146 Genova, Italy

E-mail: levi@fisica.unige.it

Received 7 July 2009 Published 14 September 2009 Online at stacks.iop.org/JPhysCM/21/405004

#### Abstract

A number of scattering situations can naively be expected to show essentially classical features, because of a (generalized) Debye–Waller factor causing decoherence and destroying interference and diffraction phenomena. It is shown, however, that such decoherence may be quenched in several ways: A—the momentum transfer to a large system may be separated into subtransfers to individual atoms, each subtransfer being too small to cause a strong Debye–Waller effect; B—(more significantly) the high-frequency vibrations may be ineffective in causing strong decoherence, because the corresponding correlation functions remain non-vanishing for too short a time. When this Debye–Waller factor quenching takes place, coherence is restored and typical quantum wave-like phenomena reappear.

### 1. Introduction

In recent years it has become increasingly clear that a number of physical phenomena, which usually appear to behave in a completely classical fashion, do so only because of decoherence [1, 2], and are ready to show quantum features as soon as the causes of decoherence are in abeyance [3]. The appearance of classical behaviour because of decoherence has been studied in great detail and has led to very interesting physics [1, 2]. Here I am interested in the opposite problem: the appearance of quantum behaviour because of the ineffectiveness of decoherence. This has also been studied, although much less often, focusing on two special cases: either the so-called 'taming of decoherence' in the context of quantum computation [4] or the quantum behaviour of relatively large objects which might naively be supposed to behave classically. I will concentrate on the latter case.

Following Zurek, someone might comment that much of what follows is not really decoherence but 'a simulation of decoherence by classical noise' [1]. In fact, I do not wish to stress entanglement, but diffraction (both are characteristically quantum phenomena; the latter, however, is simpler). The point is that wave phenomena (interference and diffraction) are *exponentially* damped by phonons, which play the role of a decoherence factor; and the return of wave phenomena when phonons, for whatever reason, are in abeyance is equally exponential and therefore very drastic. This return to coherence should not necessarily be seen as a return from classical to quantum behaviour (after all, one may consider scattering of electromagnetic radiation, in which case the coherent, wave-like behaviour is classical while the corpuscular behaviour of photons belongs to quantum physics), but in the present study I will concentrate on particle scattering: hence the return to coherence and the reappearance of interference and diffraction phenomena really amounts to a reappearance of characteristic quantum properties.

In any case, independently of whether matter or radiation is under study, decoherence in a scattering process from a solid appears primarily in terms of a *Debye–Waller factor*, which in the simplest case appears as

 $e^{-2W} = |\langle e^{i\mathbf{q}\cdot\mathbf{r}}\rangle|^2$ 

$$W = \frac{1}{2} \langle (\mathbf{q} \cdot \mathbf{r})^2 \rangle, \qquad (2)$$

(1)

where  $\hbar \mathbf{q}$  is the momentum transfer and where  $\mathbf{r}$  is a position observable which is subject to random or stochastic behaviour via its coupling to the phonon variables<sup>1</sup> (but the most interesting cases differ, in an important way, from this simplest one).

with

<sup>&</sup>lt;sup>1</sup> This is similar to the *uncontrollable measurements* discussed by Joos on page 44 of the book by Giulini *et al* [2].

#### 2. Debye–Waller factor and decoherence

In order to take a more general point of view [5, 3], let me write the differential probability for scattering of a particle from a large system into the solid angle  $d\Omega$  with energy exchange  $d\Delta$ :

$$\mathrm{d}P = \frac{A}{2\pi} \,\mathrm{d}\Omega \,\mathrm{d}\Delta \int \mathrm{e}^{-\frac{\mathrm{i}\tau\Delta}{\hbar}} \langle T_{\mathbf{k}\leftarrow\mathbf{k}_{i}}^{\dagger}(0)T_{\mathbf{k}\leftarrow\mathbf{k}_{i}}(\tau)\rangle \,\mathrm{d}\tau, \quad (3)$$

where  $T_{\mathbf{k}\leftarrow\mathbf{k}_i}$  is the *T* matrix for the particle to be scattered from wavevector  $\mathbf{k}_i$  to  $\mathbf{k}$  ( $|\mathbf{k}| = |\mathbf{k}_i|$ ); *T* is still an operator over the states of the large system, the average being taken in the initial state; and *A* is a prefactor depending on the specific scattering situation. For example, in the case of surface scattering

$$A = -\frac{L^4 m^2 k}{4\pi^2 \hbar^4 \mathbf{k}_i \cdot \mathbf{n}} \tag{4}$$

(*L* is an appropriate quantization length, *m* is the particle mass, **n** is the perpendicular unit vector out of the surface; *A* is positive because  $\mathbf{k}_i \cdot \mathbf{n}$  is negative). The time evolution of the *T* matrix in (3) is strictly related to energy exchange and has nothing to do with a different time evolution, related to the mechanism of the collision process, to be considered below. To avoid confusion, I have indicated the time variable occurring in (3) by  $\tau$ .

For *elastic* scattering into the solid angle  $d\Omega$  the differential probability is then

$$\mathrm{d}P_{\mathrm{elastic}} = A |\langle T_{\mathbf{k} \leftarrow \mathbf{k}_i} \rangle|^2 \,\mathrm{d}\Omega. \tag{5}$$

The average occurring in (5) is the same as that occurring in (1) but gives rise to a much more general Debye–Waller factor (DWF). Notice that the absolute value squared, in these formulae, must be taken *after* the average (i.e. the *T*-matrix element itself is to be averaged, not its absolute value squared).

The T-matrix element contains as its essential part a phase shift factor  $e^{i\eta}$  (in the most general case this is to be integrated over paths in a Feynman path integral [7]; in various approximations the exact and highly complex path integral is replaced by an ordinary integral, the *diffraction integral*, over the appropriate set V of variables). Understandably, the average  $\langle T \rangle$  leads thus to an average  $\langle e^{i\eta} \rangle$ , similar to (1) (this time, however, A: the latter is still to be integrated over the set of V variables, and this integration is highly relevant). Even more important (and central to my subsequent discussion) is the fact that **B**: the phase  $\eta$  itself, in general, is not a localized, or instantaneous, quantity. In what we may term the *Laue approximation*  $\eta$  would be treated as instantaneous and immediately related to the momentum transfer  $\hbar \mathbf{q}$  (a typical  $\eta$  is of the form  $\mathbf{q} \cdot \mathbf{r}$ , as in (1), where **r** is some appropriate position in the scatterer). But this Laue approximation is static and implies that such a quantity  $\mathbf{r}$  is coupled to the phonon field only via the statistics of positiona very reasonable assumption for x-rays, whose collisions take place in an exceedingly short time with respect to the phonon frequencies, but a wrong assumption in general. This has strong implications for the return to coherence.

Let me recall how the simple Debye–Waller effect (1) amounts to a decoherence. The DWF multiplies and

weakens the elastic scattering probability, which includes diffraction/interference effects, hence destroys the typical quantum nature of the scattering process. Actually, a DWF (with the appropriate changes) multiplies and weakens not only elastic scattering but also the inelastic scattering probabilities with a well-defined number of phonons exchanged [6], favouring instead the probability of random inelastic scattering. As had been shown many years ago, the resulting scattering probabilities, for a very strong DWF, tend to the classical probabilities [6]: in such a way, more or less complete decoherence is achieved. It is also important to note that (generally speaking) on increasing the mass of the colliding particle the DW effect becomes progressively more severe, and that this happens exponentially. The progressive transition from quantum to classical behaviour, due to phonon exchange, when passing from microscopic to more macroscopic objects, can thereby be explicitly followed, without any need to invoke or explore the mysticism of wavefunction collapse.

#### 3. Return to coherence

The return to coherence, in the present case, is due to some ineffectiveness of the phonon spectrum (or at least of a part of it) in generating a DWF, and thus in causing decoherence. This in turn can be traced to some reason of type **A** or, more fundamentally, of type **B** (I will concentrate on the latter, but first let me briefly discuss the former). In all cases, as shown, for example, by Feynman and Hibbs, the quantum-mechanical phase  $\eta$  equals some action *S* divided by  $\hbar$  [7]. A few properties of the action *S* will be discussed in section 4.

Leaving aside for a moment the non-instantaneous behaviour of  $\eta$ , i.e. of *S*, we may write, in the case of a particle interacting with a large system made up of individual atoms (see equation (16): below),

$$S = \hbar \sum_{n} \mathbf{q}_{n} \cdot \mathbf{r}_{n}, \qquad (6)$$

where  $\mathbf{r}_n$  is the position of the *n*th atom and  $\hbar \mathbf{q}_n$  is the momentum transfer to it (of course  $\sum_{n} \mathbf{q}_{n} = \mathbf{q}$ ). Then short-wavelength phonons (which are such that the motions of different atoms, hence the momentum transfers to them, are largely uncorrelated) are ineffective in contributing to the average  $e^{iS/\hbar}$  (provided, of course, several atoms contribute to the interaction, i.e. several  $\mathbf{q}_n$ s are non-negligible). This is an important effect of type A first studied, in particular, by Armand *et al* [8] (although the set of V variables in this case is the set of atoms, i.e. is discrete, and the integration is replaced by a sum). Such short-wavelength phonons have high frequencies, but it would be wrong to assume that high-frequency phonons are ineffective in causing decoherence because of effects of type A (optical phonons can have, of course, high frequency, but long wavelength). High-frequency phonons can really be ineffective in causing decoherence, but because of effects of type **B**, which I am now going to discuss, starting with a somewhat detailed, although elementary, consideration of the classical action S.

#### 4. The action

The standard form for the action is in terms of the Lagrangian *L*:

$$S = \int_{t_1}^{t_2} L \,\mathrm{d}t \tag{7}$$

but since L = T - V it is equally standard to write for an energy-conserving system:

$$S = \int_{t_1}^{t_2} (T - V) \, \mathrm{d}t = \int_{t_1}^{t_2} (2T - E) \, \mathrm{d}t = 2 \int_{t_1}^{t_2} T \, \mathrm{d}t - Et \quad (8)$$

where  $t = t_2 - t_1$ .

For a material point  $T = \frac{1}{2}m(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t})^2$ , so that

$$S = m \int_{t_1}^{t_2} \left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right)^2 \mathrm{d}t - Et = m \int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{v} \cdot \mathrm{d}\mathbf{r} - Et. \quad (9)$$

The integral occurring in (9) can be evaluated by parts:

$$\int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{v} \cdot d\mathbf{r} = \mathbf{v}_2 \cdot \mathbf{r}_2 - \mathbf{v}_1 \cdot \mathbf{r}_1 - \frac{1}{m} \int_{t_1}^{t_2} \mathbf{F} \cdot \mathbf{r} \, dt \qquad (10)$$

where, if **a** is the acceleration,  $\mathbf{F} = m\mathbf{a}$  is the force.

For an elastic scattering problem  $\mathbf{r}_1$ ,  $\mathbf{r}_2$ ,  $\mathbf{v}_1$ ,  $\mathbf{v}_2$  may be evaluated asymptotically, so that  $\mathbf{r}_2 = \mathbf{v}_2 t_2$  and  $\mathbf{r}_1 = \mathbf{v}_1 t_1$ , hence  $\mathbf{v}_2 \cdot \mathbf{r}_2 - \mathbf{v}_1 \cdot \mathbf{r}_1 = v_2^2 t_2 - v_1^2 t_1 = v^2 t = \frac{2E}{m} t$ ; thus

$$\int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{v} \cdot d\mathbf{r} = -\frac{1}{m} \int_{t_1}^{t_2} \mathbf{F} \cdot \mathbf{r} dt + \frac{2Et}{m}$$
(11)

and substituting into (9)

$$S = -\int_{t_1}^{t_2} \mathbf{F} \cdot \mathbf{r} \, \mathrm{d}t + Et.$$
 (12)

The second term is irrelevant for the phase shift and the action may effectively be written

$$S = -\int_{t_1}^{t_2} \mathbf{F} \cdot \mathbf{r} \, \mathrm{d}t. \tag{13}$$

In the instantaneous (or localized) case, i.e. in the *Laue* approximation, either everything takes place at a single location  $\mathbf{r}$ , which may then be extracted from the integral, obtaining

$$S = -\mathbf{r} \cdot \int \mathbf{F} \, \mathrm{d}t; \qquad (14)$$

the integral is (minus) the momentum transfer  $\Delta \mathbf{p}$ , so that  $S = \Delta \mathbf{p} \cdot \mathbf{r}$ , and quantum-mechanically

$$S = \hbar \mathbf{q} \cdot \mathbf{r}; \tag{15}$$

or, more generally, if the momentum transfer is divided among a number of scatterers,  $\mathbf{q} = \sum_{n} \mathbf{q}_{n}$ , and if scattering from the *n*th scatterer takes place when the material point is at  $\mathbf{r}_{n}$ , then

$$S = \hbar \sum_{n} \mathbf{q}_{n} \cdot \mathbf{r}_{n}, \qquad (16)$$

which coincides with equation (6). But otherwise the full equation (13) must be used.

If, instead of one material point a set of points is considered, (13) generalizes trivially to

$$S = -\sum_{i} \int_{t_1}^{t_2} \mathbf{F}_i \cdot \mathbf{r}_i \,\mathrm{d}t, \qquad (17)$$

but the force  $\mathbf{F}_i$ , acting on material point *i*, is due to the other points *j*:

$$\mathbf{F}_i = \sum_j \mathbf{F}_{ji}; \tag{18}$$

thus S can be written

$$S = -\sum_{ij} \int_{t_1}^{t_2} \mathbf{F}_{ji} \cdot \mathbf{r}_i \, \mathrm{d}t. \tag{19}$$

Let me interchange *i* with *j*:

$$S = -\sum_{ij} \int_{t_1}^{t_2} \mathbf{F}_{ij} \cdot \mathbf{r}_j \, \mathrm{d}t = \sum_{ij} \int_{t_1}^{t_2} \mathbf{F}_{ji} \cdot \mathbf{r}_j \, \mathrm{d}t \qquad (20)$$

because  $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$ . Summing (19) and (20) *S* is obtained in the form

$$S = -\frac{1}{2} \sum_{ij} \int_{t_1}^{t_2} \mathbf{F}_{ji} \cdot (\mathbf{r}_i - \mathbf{r}_j) \, \mathrm{d}t.$$
(21)

In this form *S* is the *relative* (or *mutual*) *action* and has a strong advantage over other action forms: it is *space-invariant*, since it depends only on relative coordinates, specifically on the distance  $\mathbf{r}_i - \mathbf{r}_j$ .

Independently of this, just comparing (20) with (19) it is clear that in the action it is allowed to replace  $\mathbf{r}_i$  with  $\mathbf{r}_j$  (and to change sign). In particular, let me call *i* a particle colliding with a solid and  $\mathbf{F}_i$  the force acting on it at time *t*. Then, if (as will be supposed, for example, at the beginning of section 5), the particle interacts with one atom only of the solid, whose position is  $\mathbf{r}_j$  at time *t*, (20) gives, for the part of the action involving the particle:

$$S_i = \int_{t_1}^{t_2} \mathbf{F}_i \cdot \mathbf{r}_j \, \mathrm{d}t.$$
 (22)

Although (22) is exact, its generalization to the case where the particle interacts with several atoms j:

$$S_i = \sum_j \int_{t_1}^{t_2} \mathbf{F}_i \cdot \mathbf{r}_j \, \mathrm{d}t \tag{23}$$

appears to be only an approximation. Further,  $\mathbf{r}_j$  will oscillate with the vibrational coordinates of the solid; and considering again the first approximation, i.e. neglecting the effect of vibrations on the forces, the fluctuating part of the action will be

$$\delta S_i = \sum_j \int_{t_1}^{t_2} \mathbf{F}_i \cdot \delta \mathbf{r}_j \, \mathrm{d}t, \qquad (24)$$

corresponding to a fluctuating part of the effective Lagrangian:

$$\delta L = \sum_{j} \mathbf{F}_{i} \cdot \delta \mathbf{r}_{j}.$$
 (25)

The fluctuation  $\delta L$  (not necessarily in this explicit form) will be used in section 5 to obtain the main equations of the present paper.

#### 5. Debye-Waller factor and time correlations

To discuss the (rather fundamental) effects of type **B** one may avoid the complications of type **A** considered in section 3: let me assume, for example, that the particle scatters not from a set of atoms, but just from one atom belonging to the large system. The action can simply be written, according to (13):

$$S = \int L(t) \, \mathrm{d}t = -\int \mathbf{F} \cdot \mathbf{r} \, \mathrm{d}t, \qquad (26)$$

where **r** is the position of the particle at time *t* and **F** is the force by which the atom acts on the particle. But in this case an equivalent form for the action (with a change of sign; see equation (22)) can be obtained:

$$S = \int \tilde{L}(t) \, \mathrm{d}t = \int \mathbf{F} \cdot \tilde{\mathbf{r}} \, \mathrm{d}t, \qquad (27)$$

where now  $\tilde{\mathbf{r}}$  is interpreted as the position *of the atom* at time *t*. Noise arises from the fact that both  $\mathbf{F}$  and  $\tilde{\mathbf{r}}$  are randomly affected by the phonons. Thus  $S = S_0 + \delta S$  and only the random part  $\delta S$  matters for the DWF (similarly  $\tilde{L}(t) = \tilde{L}_0(t) + \delta L(t)$ ). *S* and  $\eta$  are thus integrals over collision time and, when taking the average of the *T*-matrix element, we have

$$\langle e^{\frac{i}{\hbar}S} \rangle = \langle e^{\frac{i}{\hbar}\int \tilde{L}(t)\,dt} \rangle = e^{\frac{i}{\hbar}\int \tilde{L}_0(t)\,dt} \langle e^{\frac{i}{\hbar}\int \delta L(t)\,dt} \rangle.$$
(28)

The random contributions in the last integral are (to a first approximation, in particular neglecting the effect of phonons on the forces<sup>2</sup>, and considering only the effect of phonons on the displacements) linear in the phonon variables, and the latter have a Gaussian distribution. Therefore, the above contributions also have a Gaussian distribution and I can use the elementary theorem for Gaussian variables with zero average (also valid, although in a less elementary way, for Gaussian quantum operators):

$$\langle e^{i\alpha} \rangle = e^{-\frac{1}{2} \langle \alpha^2 \rangle}.$$
 (29)

Thus

$$\begin{aligned} |\langle \mathbf{e}^{\frac{\mathbf{i}}{\hbar}S} \rangle|^2 &= |\mathbf{e}^{\frac{\mathbf{i}}{\hbar}\int \tilde{L}_0(t)\,\mathrm{d}t} \,\langle \mathbf{e}^{\frac{\mathbf{i}}{\hbar}\int \delta L(t)\,\mathrm{d}t} \rangle|^2 = |\langle \mathbf{e}^{\frac{\mathbf{i}}{\hbar}\int \delta L(t)\,\mathrm{d}t} \rangle|^2 \\ &= |\mathbf{e}^{-\frac{1}{2\hbar^2}\langle [\int \delta L(t)\,\mathrm{d}t]^2 \rangle}|^2 = \mathbf{e}^{-\frac{1}{\hbar^2}\langle [\int \delta L(t)\,\mathrm{d}t]^2 \rangle}. \end{aligned}$$

The DWF is thus

$$e^{-2W}, \qquad W = \frac{1}{2\hbar^2} \left\langle \left[ \int \delta L(t) \, \mathrm{d}t \right]^2 \right\rangle.$$
 (30)

The most important point here is that the DWF is related to the correlation between Lagrangians *at different times*. Indeed *W* can be rewritten as

$$W = \frac{1}{2\hbar^2} \left\langle \int \delta L(t) \, \mathrm{d}t \int \delta L(t') \, \mathrm{d}t' \right\rangle,$$

i.e. interchanging integration and average:

$$W = \frac{1}{2\hbar^2} \int \int \langle \delta L(t) \delta L(t') \rangle \, \mathrm{d}t \, \mathrm{d}t'. \tag{31}$$

<sup>2</sup> This is allowed, for example, for slowly varying potentials, but is exact again for abrupt potentials: complications may arise only in intermediate situations.

The double integral converges in all cases because both  $\delta L$ 's are to be considered within the collision time  $\tau_c$  only; but if, moreover, the correlation function, related to the phonon vibrations, vanishes whenever  $|t' - t| \gg \tau_{ph}$ , then *W* becomes small when  $\tau_{ph}$  is short, i.e. for relatively high phonon frequencies.

For the return to coherence formula (31) is very relevant. Indeed in the present case decoherence takes place with increasing mass of the incoming particle simply because for given accelerations in the scattering potential the forces, and hence the Lagrangians, increase with the mass, leading rapidly (*W* appears in the exponent!) to classical behaviour. This is true for given accelerations, i.e. for given collision times, but remains valid whenever the phonon frequencies are so low (or the particle motion so fast) that the whole collision appears to be instantaneous with respect to the phonon oscillations. In the opposite case, however, (31) must be taken seriously.

The most important consequence of (31) is that a heavy particle may show quantum-mechanically coherent behaviour because its collision requires a long time to be completed, while the correlation function (related to the phonon oscillations) vanishes in a much shorter time. Or, in a slightly different language, by the adiabatic principle, highfrequency phonons cannot easily be excited (or de-excited) in a long, slow collision. This leads to a relatively small value of W, and hence to relatively strong quantum-mechanical effects<sup>3</sup>. Counting times from the central instant of the collision, let me assume, for example, that the correlation function occurring in (31) behaves as

$$\langle \delta L(t) \delta L(t') \rangle \sim \langle [\delta L(0)]^2 \rangle \mathrm{e}^{-\alpha(|t|+|t'|)-\beta|t'-t|},\tag{32}$$

where  $\alpha = \tau_c^{-1}$ ,  $\beta = \tau_{ph}^{-1}$ . Then

$$W = \langle [\delta L(0)]^2 \rangle \frac{\tau_{\rm ph} \tau_{\rm c}^2}{\hbar^2} \frac{2\tau_{\rm ph} + \tau_{\rm c}}{(\tau_{\rm ph} + \tau_{\rm c})^2},$$
(33)

i.e.

$$W \sim p\tau_{\rm c}^2 \frac{\langle [\delta L(0)]^2 \rangle}{\hbar^2} \tag{34}$$

if  $\tau_{\rm ph} \gg \tau_{\rm c}$  and

$$W \sim q \tau_{\rm ph} \tau_{\rm c} \frac{\langle [\delta L(0)]^2 \rangle}{\hbar^2}$$
(35)

if  $\tau_{\rm ph} \ll \tau_{\rm c}$ , with p = 2, q = 1. The exponential expression used in (32) is largely irrelevant: with any other simple, reasonable behaviour (34) and (35) would equally obtain (only the coefficients p and q would possibly be different). Thus W turns out to be essentially independent of  $\tau_{\rm ph}$  if the latter is large (low phonon frequencies), but reduces proportionally to  $\tau_{\rm ph}$  if the latter becomes short (i.e. if the phonon frequencies are high with respect to relatively slow collisions).

 $<sup>^{3}</sup>$  In some cases, as shown by Beeby, for a light particle the opposite happens (due to acceleration in the potential well) and *W* increases [9]; this complication is irrelevant here.

#### 6. Experimental results

An interesting, recent application of the effects of type A is grazing incidence fast atom diffraction (GIFAD) [10], where, due to grazing incidence, several successive atoms participate in the scattering, each receiving a very small momentum transfer. Turning now to the effects of type B, the first experimental results related to the above were obtained many years ago in our university by Boato et al In atomsurface scattering. The most prominent quantum effects are diffractions from the crystal lattice: these had been observed with hydrogen and helium scattering already around 1930 by Stern's group in Hamburg [11] and independently by Johnson [12] (at the time, these experiments were seen as rather fundamental, proving the quantum behaviour of complex systems such as atoms). With neon atoms, on the other hand, nothing similar was expected and elementary estimates indicated that the exponential DWF was going to kill any diffraction. In contrast, with some surprise, Boato et al studying the scattering of Ne from a LiF surface saw a set of beautiful diffraction peaks (although less sharp than those of He) [13].

Recently, on the other hand, the Cambridge group has studied the scattering of Ne from a different system: an adsorbate of Li forming a  $c(2 \times 2)$  structure on the (100) surface of copper. Quantum behaviour appeared again (high reflectivity and diffraction peaks), but this time much more strongly than in Boato's case: neon showed quantum features as sharp as those of helium [14].

These experiments, showing unexpected coherence in relatively heavy atom scattering, have easily been explained [5, 3] on the basis of the concepts discussed above. It is also understandable why the effect found by the Cambridge group was stronger than that found by the Genova group: this depends on the different phonon spectra in the two cases. The effect occurs because high-frequency phonons cannot be excited during a slow collision process. Lithium fluoride is a bulk system possessing a normal spectrum, with a sizeable contribution of low frequencies. If for such spectrum a Debye model is assumed, W can be shown to increase with mass, although less than in the elementary case (as  $\sqrt{m}$  instead of as m [5]): thus for Boato neon appeared unavoidably to be less quantum-mechanical than helium. But the lithium adsorbate has a spectrum dominated by a single, relatively high, frequency, that of the perpendicular motion of Li atoms against the Cu surface: in this case the dominant frequency has no effect (its contribution to W would be paradoxically less for neon than for helium!) and the quantum-mechanical behaviour of the two atoms can be similar [3].

#### 7. Discussion

With the support of these experimental facts, I wish to turn now to the conceptual significance of the discussion. Although previous papers [5, 3] have been instrumental in exploring the effects of slow atoms colliding with solids possessing a high-frequency spectrum, and have explained theoretically in detail the experimental facts concerning neon scattering, the

core of the matter remained somewhat hidden: the present paper is aimed not only at clarifying such a core, but also at showing that very general principles, lying at the border between classical and quantum physics, are involved. At first sight, the DWF might appear as a very special effect, related to solid state physics; but in fact I think it to be a convincing example of a large class of decoherence effects. Quantum coherence is obviously related to the phase of the wavefunction and, as in equation (1) or in equations (30)–(31), Gaussian disturbances of any kind (not necessarily phonons!) cause an averaging of the phase factor which in turn results in an exponential reduction of the coherent terms. Such disturbances increase rapidly when passing to more macroscopic situations (or, in the above discussion, to a heavier scattering particle) and decoherence takes place exponentially. I am not claiming that this explains the whole transition from quantum to classical behaviour when passing from microscopic to macroscopic objects (I have left aside the subtle effects of entanglement, on which a rich and far from trivial literature exists, showing that simplified treatments tend to miss the goal [1, 2]). But much of this transition is nothing but an averaging of phase factors, as indeed can be surmised from the simplest examples presented by Zurek [1].

On the other hand, return to coherence occurs when, for any reason, the effect of disturbances is reduced. In the above discussion, a large number of atoms contributing to the scattering is, perhaps surprisingly, less effective for decoherence than a single atom, because each receives a small portion only of the momentum transfer (effect of type **A**); or the increase of disturbance with increasing particle mass is weak because at the same time, as in (31), a correlation remains non-vanishing only for times much shorter than the duration of the collision (effect of type **B**). Thus one might expect that the hope of seeing quantum properties with relatively large objects resides ultimately in reducing the disturbances causing decoherence, which is hardly surprising.

According to Feynman's philosophy, quantum amplitudes are obtained by weighting a phase factor  $e^{iS/\hbar}$ , where *S* is any possible action, over a space of quantum paths [7], while the classical limit obtains when only the minimal (or rather extremal) action  $S_{cl}$  is taken into account. Even quantummechanically,  $S_{cl}$  necessarily yields the largest contribution by the principle of stationary phase, while the contribution of any specified action different from it (and thus non-extremal) is attenuated, its average leading to a generalized DWF similar to (30)–(31). If the effects of such a DWF happen to be weak, e.g. for the reasons discussed in the present paper, nonextremal actions become important and typical quantum wavelike phenomena reappear.

#### Acknowledgments

The author is grateful to Professor C M Becchi for critical reading of the manuscript, in particular for pointing out an essential role of the time evolution. In (3) and (31) conceptually different time variables are indicated, respectively, by  $\tau$  and by t, t'.

#### References

- [1] Zurek W H 2003 Rev. Mod. Phys. 75 715
- [2] Giulini D, Joos E, Kiefer C, Kupsch J, Stamatescu I-O and Zeh H D 1996 Decoherence and the Appearance of a Classical World in Quantum Theory (Berlin: Springer)
- [3] Levi A C, Huang C, Allison W and MacLaren D A 2009 J. Phys.: Condens. Matter 21 225009
- [4] Zanardi P 1998 Phys. Rev. A 57 3276
  Zanardi P 2001 Phys. Rev. A 63 012301
- [5] Levi A C and Suhl H 1979 Surf. Sci. 88 221
- [6] Levi A C 1979 Nuovo Cimento B 54 357
- [7] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
- [8] Armand G, Lapujoulade J and Lejay Y 1976 J. Phys. Lett. 37 L187

Armand G, Lapujoulade J and Lejay Y 1977 Surf. Sci. 63 143

A C Levi

- [9] Beeby J L 1971 J. Phys. C: Solid State Phys. 4 L359
- [10] Rousseau P, Khemliche H, Borisov A G and Roncin P 2007 Phys. Rev. Lett. 98 016104
  - Manson J R, Khemliche H and Roncin P 2008 *Phys. Rev.* B 78 155408
- [11] Estermann I and Stern O 1930 Z. Phys. 61 95
  Estermann I, Frisch R and Stern O 1931 Z. Phys. 73 348
  Frisch R and Stern O 1933 Z. Phys. 84 430
- [12] Johnson T H 1930 J. Franklin Inst. 210 135
- [13] Boato G, Cantini P, Garibaldi U, Levi A C, Mattera L, Spadacini R and Tommei G E 1973 J. Phys. C: Solid State Phys. 6 L394
  - Boato G, Cantini P and Mattera L 1976 Surf. Sci. 55 141
- [14] MacLaren D A, Huang C, Levi A C and Allison W 2008
  *J. Chem. Phys.* **129** 094706