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Phase uncertainty and loss of interference in a simple model for mesoscopic Aharonov-Bohm experiments

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Incoherence introduced in two-path experiments by interactions with scatterers in thermal equilibrium is examined with an energy-momentum approach previously used for the Mössbauer effect. Oscillations in intensity with variations in the magnetic flux are shown to be insensitive to random phase changes in the individual scattering amplitudes. Inelastic incoherent scattering may be suppressed when there are a large number of scatterers. A small loss of phase coherence negligible in cases of practical interest can occur even via elastic scattering, which does not perturb the environment. The temperature dependence of the loss of interference, analogous to the Debye-Waller factor, may be tested by experiment.

I. INTRODUCTION: A SIMPLE SINGLE SCATTERER MODEL

The suppression of quantum interference due to the coupling of the interfering degrees of freedom to many other degrees of freedom has always been a central subject in the understanding of quantum phenomena.[1] Its importance has recently been emphasized in experiments on mesoscopic systems.[2] While most treatments of these effects use a space-time description, the equivalent complementary energy-momentum description often provides useful insight from a different point of view.[3–8] We examine the possible use of this approach here.

Consider one of the Aharonov-Bohm experiments[9] in which an electron can go in two paths around a ring which contains magnetic flux, and the relative phase of the two waves depends upon the flux.[2] Let a scatterer like an impurity ion bound in some potential in a state of thermal equilibrium be put at one point on the ring so that one path goes by the scatterer and the other does not. The scattering process will be either elastic—like the Mössbauer effect—with the scatterer remaining in the same bound state after the scattering, or inelastic, with a change in the state of the scatterer.[5] The elastically scattered wave is coherent with the wave going through the other path and shows the Aharonov-Bohm coherence and interference effects. The inelastically scattered component is not coherent and does not interfere with the component from the other path. This can be seen formally by expanding the total electron-scatterer wave function in a factorized basis and integrating over the scatterer variables. The elastic amplitudes all have the scatterer in the same state. Thus the integral over the scatterer variables in the interference term between any two elastic amplitudes gives a factor of unity. The interference terms between an elastic and an inelastic amplitude vanish when integrated over the scatterer variables, because the two amplitudes have the scatterer in two different orthogonal states.

The intensity of the scattered wave in a transition where the scatterer goes from an initial state $|i\rangle$ to a final state $|j\rangle$ is proportional to the square of a matrix element which depends upon the momentum transfer and thus on the angular distribution of the scattered wave,

$$f_{i\to j}=|\langle j|e^{i\delta\mathbf{k}\cdot\mathbf{x}}|i\rangle|^2 , \tag{1a}$$

where $\delta\mathbf{k}$ is the momentum transfer during the scattering process and $\mathbf{x}$ is the distance between the position of the scatterer and its equilibrium position. This factor arises in many different areas of physics in which there is a momentum transfer to bound systems. The matrix element (1a) is often called a form factor or structure factor. The square is called the Debye-Waller or Mössbauer fraction factor. The form factor satisfies the well-known sum rule

$$\sum_j f_{i\to j}=\sum_j |\langle j|e^{i\delta\mathbf{k}\cdot\mathbf{x}}|i\rangle|^2=1 . \tag{1b}$$

The scattered intensity is the product of three factors, the Debye-Waller factor $f_{i\to j}$, a factor depending upon the details of the scattering process from a free scatterer, and a phase-space factor. The basic physical assumption underlying this factorization is the impulse approximation,[3,8] in which the bound-state scatterer wave function is expanded in a plane-wave basis and the scattering operator is applied separately to each plane-wave component. This assumption is trivially valid in all scattering processes treated in Born approximation. A general derivation is given in the Appendix below.

The Debye-Waller factor for the case of a single elastic scattering from a single impurity subject to thermal and zero-point oscillations in the lattice is given by Eq. (1a) as

$$f_1=\sum_i P_i|\langle i|e^{i\delta\mathbf{k}\cdot\mathbf{x}}|i\rangle|^2 , \tag{2a}$$

where P_i denotes the probability that the scatterer is in the state $|i\rangle$.

In the Mössbauer effect all the dependence of the scattering cross section on the properties of the bound state is given by the Debye-Waller factor (1). The γ-ray energy is very much larger than the excitation energies in the scatterer system; thus the phase-space factor is the same for all relevant inelastic final states to an excellent approximation and the dependence of the scattering from a free scatterer on the velocity of the scatterer is negligible over the domain of zero-point and thermal velocities. For this case the sum rule (1b) shows that the Debye-Waller factors (1a) gives the normalized relative probabilities for each transition, f_1 is equal to the elastic scattering probability and a difference between f_1 and unity indicates the presence of incoherent inelastic scattering.

This probability interpretation breaks down if there is a significant energy loss in the dominant inelastic transitions. The phase-space factor is then lower for these inelastic transitions. The Debye-Waller factor f_1 still appears in the expression for the elastic cross section, but no longer as a normalized probability. It is only a lower bound for the elastic scattering probability and the difference between f_1 and unity no longer indicates the presence of incoherent inelastic scattering. This is easily seen in the extreme case where the excitation energy of the first excited state of the scatterer is greater than the electron energy. Inelastic scattering is energetically forbidden; all scattering is elastic and coherent, but the form factor appears in the elastic cross section and has a very simple physical interpretation. It is the Fourier transform of the probability density of the thermal and zero-point motion. It expresses the fact that the scatterer appears as a finite density distribution at energies small compared to the characteristic energy of its motion.[3,8]

Evaluating the matrix elements in (2a) and summing over the probability distribution P_i give the well-known result,

$$f_1 \approx e^{-\langle(\delta\mathbf{k}\cdot\mathbf{x})^2\rangle} \approx e^{-(\delta k)^2\langle x_{\delta k}^2\rangle} , \tag{2b}$$

where $\langle x_{\delta k}^2\rangle$ is the mean-square deviation in the direction of $\delta\mathbf{k}$ of the oscillating scatterer from its equilibrium position averaged over the distribution.

This result is valid in nearly all cases of practical interest. It has two independent derivations:[10] (1) as an exact result for the case of a harmonic oscillator at zero temperature, i.e., for a scatterer wave function with a Gaussian probability density in configuration space; (2) as a lowest-order result in powers of the momentum transfer $\delta\mathbf{k}$ for the general case, as can be seen by expanding the exponential in Eq. (1a). It is better than a lowest-order approximation for most reasonable potentials, since the difference between the higher-order terms in the expansions (1a) and (2b) vanishes for a Gaussian density and therefore depends only on the difference between the actual density and a Gaussian. In cases of practical interest, there are many scatterers, and the elastic amplitude involves the product of many Debye-Waller factors. The total elastic amplitude will therefore be appreciable only when all these factors are reasonably close to unity and the lowest-order result is a very good approximation.

The role of the Debye-Waller factor in phase coherence has also been pointed out[11] with reference to a discussion of dephasing of weak localization by zero-point motion.[12] That this issue is irrelevant to the Aharonov-Bohm phases in the experiments under discussion is shown in detail below.

II. A MODEL WITH A LARGE NUMBER OF SCATTERERS

A. The case of a single elastic amplitude

We now generalize this model by introducing a large number of scatters. We first consider the case where the elastic scattering amplitude can be expressed as a single amplitude which is proportional to the product of the square roots of all the Debye-Waller factors, one for each scatterer. For the case where the elastic scattering intensity is appreciable, each of these factors must be individually close to unity and the approximation (2b) can be used. The intensity of the observed elastic scattering then depends upon the product of a large number of Debye-Waller factors.

$$F=\prod_i f_i=\exp\left[-\sum_i\langle(\delta\mathbf{k}_i\cdot\mathbf{x}_i)^2\rangle\right] =\exp\left[-\sum_i \delta k_i^2\langle x_i^2\rangle\right] , \tag{3}$$

where F denotes the overall Debye-Waller factor for elastic scattering from a large number of impurities and $\delta\mathbf{k}_i$ and $\langle x_i^2\rangle$ are the momentum transfer and the mean-square deviation in the direction of $\delta\mathbf{k}_i$ of the oscillating scatterer for each individual scattering process labeled by the index i. This overall factor can be expressed in terms of lattice properties which depend upon the temperature, phonon variables, Debye temperatures, etc. For a system in thermal equilibrium at a temperature T

$$F(T)\approx\exp\left[-\frac{R}{\hbar\omega}\coth\frac{\hbar\omega}{2kT}\right] , \tag{4a}$$

where ω is an average characteristic frequency for the motion of the scatterer in the lattice,

$$R=\sum_i \hbar^2\delta k_i^2/2M , \tag{4b}$$

where M is the mass of the scatterer, and we have used the value for a single harmonic oscillator in thermal equilibrium,

$$\langle x_i^2\rangle=\frac{\hbar}{2M\omega}\coth\frac{\hbar\omega}{2kT} . \tag{4c}$$

For the case where the motion of the scatterers is described by a Debye model of the crystal, the expression (3) is a well-defined known function of the temperature and of the Debye temperature Θ of the crystal. At zero temperature the Debye model gives

$$F(0)=\exp\left[-\frac{3R}{2k\Theta}\right] . \tag{5}$$

Thus in a model where the destruction of interference by inelastic scattering comes from systems of oscillators in thermal equilibrium[6] the signal should be suppressed by something like a Debye-Waller factor [(4) and (5)] which should show a characteristic temperature dependence, possibly related to known bulk properties of the solid, such as a Debye temperature. This could be tested by experiment.

The evaluation of the Debye-Waller factors (3) depends upon the details of the scattering processes and the individual momentum transfers $\delta\mathbf{k}_i$. One can envision many different scattering contributions, each defined by a different set of values of $\delta\mathbf{k}_i$ and each having a different Debye-Waller factor. Although a quantitative treatment for this case is not feasible, qualitative factors indicate that the process may be dominated by very low values of δk_i; i.e., forward scattering, where the Debye-Waller factors are close to unity. The forward-scattered intensity can also be enhanced by coherence factors of the order $N^{(1/3)}$ where N is the number of scatterers.[13-15] Such coherence effects have been observed in γ-ray scattering by ions in crystals[16,17] and should also be present in electron scattering. This coherence enhancement reduces the loss due to inelastic processes by the $N^{(1/3)}$ factor which may be appreciable.

B. The case of many incoherent elastic amplitudes

A more realistic model considers contributing amplitudes, each describing a transition in which the electron interacts differently with some set of a large number of scatterers; e.g., a multiple-scattering expansion in which there is a single-scattering amplitude, a double-scattering amplitude, etc. We need not specify the details of these individual amplitudes, but simply label them as a_n where $1 \le n \le N_a$ for the set of elastic amplitudes which traverse paths going around the magnetic flux in one direction and b_n where $1 \le n \le N_b$ for the set going around in the other direction. We assume that N_a and N_b are both large and that all these amplitudes have random phases with respect to one another, except that the relative phase between any a_m amplitude and any b_n amplitude depends upon the magnetic flux Φ in the ring in a manner independent of m and n. The amplitudes thus satisfy the conditions

$$a_m^* a_n = A_{mn} \ , \quad (6a)$$

$$b_m^* b_n = B_{mn} \ , \quad (6b)$$

$$a_m^* b_n = e^{i\eta(\Phi)} G_{mn} \ , \quad (6c)$$

where the phase $\eta(\Phi)$ depends upon the magnetic flux Φ, while A_{mn}, B_{mn}, and G_{mn} depend upon m and n and are independent of the magnetic flux. Thus the intensity observed in the experiment depends upon the magnetic flux only via the interference between the a and b amplitudes,

$$\begin{aligned} I &= \left| \sum_m a_m + \sum_n b_n \right|^2 \\ &= \left| \sum_m a_m \right|^2 + \left| \sum_n b_n \right|^2 \\ &\quad + \sum_{m,n} \left(e^{i\eta(\Phi)} G_{mn} + e^{-i\eta(\Phi)} G_{mn}^* \right) . \end{aligned} \quad (7)$$

Let us assume that $N_a \approx N_b \equiv N \gg 1$. Then if all the terms in the various summations have random phases,

$$\sum_m |a_m^2| = N\langle |a^2| \rangle \ , \quad (8a)$$

$$\sum_m |b_m^2| = N\langle |b^2| \rangle \ , \quad (8b)$$

$$\left| \sum_m a_m \right|^2 = N\langle |a^2| \rangle + [N(N-1)]^{1/2} \langle |a| \rangle^2 \ , \quad (8c)$$

$$\left| \sum_n b_n \right|^2 = N\langle |b^2| \rangle + [N(N-1)]^{1/2} \langle |b| \rangle^2 \ , \quad (8d)$$

$$\left| \sum_{m,n} G_{mn} \right| = N\langle |ab| \rangle \ , \quad (8e)$$

where $\langle |a| \rangle$, $\langle |b| \rangle$, $\langle |a^2| \rangle$, $\langle |b^2| \rangle$, and $\langle |ab| \rangle$ denote average values of these quantities. Let us define a phase θ by the relation

$$\sum_{m,n} G_{mn} \equiv \left| \sum_{m,n} G_{mn} \right| e^{-i\theta} \ . \quad (8f)$$

Then to leading order in N,

$$\begin{aligned} I &\approx N\langle |a^2| \rangle + N\langle |a| \rangle^2 + N\langle |b^2| \rangle + N\langle |b| \rangle^2 \\ &\quad + 2N\langle |ab| \rangle \cos[\eta(\Phi) - \theta] \ . \end{aligned} \quad (9)$$

Thus the elastic contribution to the intensity contains a term oscillating with the magnetic flux of the same order as the term independent of the flux, and this result is independent of any effects in the solid which might change the relative phases of the individual a_m and b_n amplitudes.

III. POSSIBLE LOSS OF COHERENCE IN ELASTIC SCATTERING

So far we have considered all elastic scattered amplitudes as coherent, and have not examined the possibility of a loss of phase coherence in elastic scattering. This approach is justified when the scatterers are in a pure quantum state. However, if the scatterers are described by a statistical mixture; e.g., an ensemble in thermal equilibrium, there can be a loss of phase coherence. One indication of such a loss is the dependence of the expression (9) upon the particular quantum state of the scatterer system via a parameter θ. If the scatterer is described by a statistical mixture of states, each having a different value of θ, the oscillations of the intensity with magnetic flux can average out, and the effect can be lost.

This effect can be seen in a simple model with a single scatterer in the a path and no scatterer in the b path. Let the scatterer be an impurity atom with energy levels such that the Debye-Waller factor is unity for the ground state and zero for all other states. This could be achieved if the potential consists of a strong attraction with very short-range and a much weaker long-range attraction such that there is only one bound state in the short-range potential. Let P_g denote the probability that the scatterer is in the ground state, and let a_0 and a_1, denote, respectively the contributions to the amplitude when the electron goes through path a without being scattered and with being scattered by the scatterer. Then the intensity observed in the experiment is given by modifying Eqs. (7)–(9) to give an incoherent sum of the intensities corresponding to the case where the scatterer is in its ground state and when it is not in its ground state:

$$I=|a_0|^2+|b|^2+P_g|a_1|^2+2P_g|a_0a_1|\cos(\theta_0-\theta_1)$$
$$+2|a_0b|\cos[\eta(\Phi)-\theta_0]$$
$$+2P_g|a_1b|\cos[\eta(\Phi)-\theta_1]\ , \tag{10a}$$

where θ_0 and θ_1 are defined by the analog of Eq. (8d)

$$a_0^*b\equiv e^{i\eta(\Phi)}|a_0b|e^{-i\theta_0}\ , \tag{10b}$$

$$a_1^*b\equiv e^{i\eta(\Phi)}|a_1b|e^{-i\theta_1}\ . \tag{10c}$$

A certain loss of coherence is seen in the appearance of two periodic functions with a phase difference between them.

We now generalize this treatment to the case of an arbitrary number of identical scatterers in thermal equilibrium each having a probability denoted by P_i for being in a state denoted by i which has a Debye-Waller factor denoted by f_i, but only single-scattering amplitudes are considered. We generalize Eqs. (6) and (7) by redefining the amplitudes a_m and b_m as reduced amplitudes without the Debye-Waller factors, so that the scattering amplitude from scatterer m in the state i is given by $\sqrt{f_i}a_m$. For this case Eq. (7) becomes

$$I=\sum_i P_i f_i\left[\left|\sum_m a_m\right|^2+\left|\sum_n b_n\right|^2\right]+\sum_{i,j}P_iP_j(f_if_j)^{1/2}$$
$$\times\left[\sum_{m\neq n}(A_{mn}+A^*_{mn}+B_{mn}+B^*_{mn})+\sum_{m,n}(e^{i\eta(\Phi)}G_{mn}+e^{-i\eta(\Phi)}G^*_{mn})\right]\ . \tag{11a}$$

This can be rewritten

$$I=\langle f\rangle\left[\left|\sum_m a_m\right|^2+\left|\sum_n b_n\right|^2\right]$$
$$+\langle\sqrt{f}\,\rangle^2\left[\sum_{m\neq n}(A_{mn}+A^*_{mn}+B_{mn}+B^*_{mn})+\sum_{m,n}(e^{i\eta(\Phi)}G_{mn}+e^{-i\eta(\Phi)}G^*_{mn})\right]\ , \tag{11b}$$

where $\langle f\rangle$ and $\langle\sqrt{f}\,\rangle$ denote the thermal averages of these factors.

The interference terms including the interesting term which depends upon the magnetic flux are seen to be suppressed by a factor $\langle\sqrt{f}\,\rangle^2$ while the direct terms are suppressed by the factor $\langle f\rangle$. Since $0\le f_i\le 1$,

$$\langle f\rangle\ge\langle\sqrt{f}\,\rangle^2\ge\langle f\rangle^2\ , \tag{12a}$$

$$1\ge\frac{\langle\sqrt{f}\,\rangle^2}{\langle f\rangle}\ge\langle f\rangle\ . \tag{12b}$$

That the interference terms are suppressed by a larger factor than the direct terms shows the loss of coherence or the introduction of phase uncertainty as a result of the coupling of the scatterers to a heat bath which keeps the scatterers in thermal equilibrium. However, the ratio of the suppression factors of the interference and direct terms is less than the suppression factor for the total elastic scattering contribution. This suggests that the effect of loss of phase coherence in elastic scattering cannot be serious in any practical experiment. The loss of phase coherence is appreciable only when the elastic amplitude itself is very small, having been drastically reduced by the Debye-Waller factor.

Although the restriction to only single-scattering contributions is an oversimplification, the model seems to show a general property that the loss of phase coherence arises from incoherent excitations of states with Debye-Waller factors. Since these factors are always less than one, the total elastic scattering from such states is also correspondingly reduced and the phase coherence loss is appreciable only when the elastic scattered intensity is reduced by a large factor.

The result (12) has a simple physical interpretation. The density matrix of a thermal distribution has no off-diagonal matrix elements in a basis of energy eigenstates. Thus the result of any experiment is thus a weighted average of the results of experiments performed with pure energy eigenstates. From Eq. (9) we see that the only dependence of the result on the particular energy eigenstate is in the Debye-Waller factors. Thus coherence can be lost by thermal averaging only when the states dominating the thermal distribution have significantly different Debye-Waller factors; i.e., have factors much smaller than unity. This case is not expected to be important in practical experiments.

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APPENDIX: GENERAL DERIVATION OF THE FORM FACTOR (1)

The transition matrix element for the scattering of an electron of momentum $\mathbf{p}_e$ and a momentum transfer $\delta\mathbf{k}$ by a scatterer which goes from an initial state $|i\rangle$ to a final state $|j\rangle$ can be simplified by expanding the states $|i\rangle$ and $|j\rangle$ in a plane-wave basis denoted by $|\mathbf{k}\rangle$

$$\langle j|T(\mathbf{p}_e,\delta\mathbf{k})|i\rangle=\sum_{\mathbf{k},\mathbf{k}'}\langle j|\mathbf{k}'\rangle\langle\mathbf{k}'|T(\mathbf{p}_e,\delta\mathbf{k})|\mathbf{k}\rangle\langle\mathbf{k}|i\rangle\ . \tag{A1a}$$

If momentum conservation is assumed in the scattering process, only the terms in which $\mathbf{k}'=\mathbf{k}+\delta\mathbf{k}$ are nonvanishing and

$$\langle j|T(\mathbf{p}_e,\delta\mathbf{k})|i\rangle=\sum_{\mathbf{k}}\langle j|\mathbf{k}+\delta\mathbf{k}\rangle t(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})\times\langle\mathbf{k}+\delta\mathbf{k}|e^{i\delta\mathbf{k}\cdot\mathbf{x}}|\mathbf{k}\rangle\langle\mathbf{k}|i\rangle\ , \quad \text{(A1b)}$$

where $t(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})$ denotes the transition matrix element in the plane-wave basis. The conventional result with the Debye-Waller factor (1) now follows from the additional assumption that the dependence of $t(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})$ on $\mathbf{k}$ can be neglected over the domain of $\mathbf{k}$ relevant to the bound-state wave function of the scatterer. In this approximation the summation over $\mathbf{k}$ by closure gives

$$\langle j|T(\mathbf{p}_e,\delta\mathbf{k})|i\rangle\approx t_{\mathbf{k}}(\mathbf{p}_e,\delta\mathbf{k})\langle j|e^{i\delta\mathbf{k}\cdot\mathbf{x}}|i\rangle\ , \quad \text{(A2)}$$

where $t_{\mathbf{k}}(\mathbf{p}_e,\delta\mathbf{k})$ denotes the value of $t(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})$ at some appropriate value of $\mathbf{k}$.

We now examine the validity of the two approximations used. Neglecting the dependence of $t(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})$ on $\mathbf{k}$ appears to be a reasonable, since $t(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})$ is expected to be a smoothly varying function of the relative velocity between the electron and the scatterer

$$\mathbf{v}_{\text{rel}}=\frac{1}{m}\left(\mathbf{p}_e-\frac{m}{M}\mathbf{k}\right)\approx\frac{\mathbf{p}_e}{m}\left[1-\frac{m}{M}\frac{\mathbf{k}\cdot\mathbf{p}_e}{p_e}\right] \quad \text{(A3a)}$$

and the ratio of the electron mass m to the scatterer mass M is a very small number. Thus

$$\frac{dt(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})}{dk}=\frac{dt(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})}{dv_{\text{rel}}}\frac{dv_{\text{rel}}}{dk}=-\frac{m}{M}\frac{\mathbf{k}\cdot\mathbf{p}_e}{kp_e}\frac{dt(\mathbf{p}_e,\mathbf{k},\delta\mathbf{k})}{dp_e}\ . \quad \text{(A3b)}$$

We now examine the assumption of momentum conservation. If the electron-scatterer interaction conserves momentum, the T matrix also conserves momentum in Born approximation and the impulse approximation (A1b) is valid. In higher orders in the perturbation series, the propagators of intermediate bound states of the scatterer do not conserve momentum, and there can be corrections to the simple Debye-Waller factor (1).

Most treatments of these phenomena do not go beyond the Born approximation. We shall now see in a simple example how a higher-order correction does not affect our conclusions in cases where the relevant Debye-Waller factors are not very different from unity. Consider the generalization of Eq. (A1) to treat an elastic double-scattering contribution with momentum transfers $\delta\mathbf{k}_\alpha$ and $\delta\mathbf{k}_\beta$ from an initial scatterer state $|i\rangle$ with energy E_i via an intermediate state $|j\rangle$ with energy E_j;

$$\langle i|T^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)|i\rangle=\sum_{j\neq i}\frac{t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{E_i-E_j}\times\langle i|e^{i\delta\mathbf{k}_\alpha\cdot\mathbf{x}}|j\rangle\times\langle j|e^{i\delta\mathbf{k}_\beta\cdot\mathbf{x}}|i\rangle\ , \quad \text{(A4)}$$

where the reduced t matrix $t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)$ depends only on the momenta and is independent of the properties of the scatterer bound states. For simplicity we assume that the system is isotropic and discard all anisotropic contributions to the expression (A4).

In cases where the Debye-Waller factors are not too small, this expression can be approximated by the leading term in the expansion in powers of $\delta\mathbf{k}_\alpha$ and $\delta\mathbf{k}_\beta$;

$$\langle i|T^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)|i\rangle\approx\sum_{j\neq i}\frac{t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{E_j-E_i}\times\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta|\langle i|x_\alpha|j\rangle|^2\ , \quad \text{(A5a)}$$

where x_α denotes the component of $\mathbf{x}$ in any given direction; e.g., the direction of k_α. Since $|\langle i|x_\alpha|j\rangle|^2$ is positive definite we can obtain an inequality by replacing the energy denominators by their minimum value and summing by closure,

$$|\langle i|T^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)|i\rangle|\leq\left|\frac{t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{E_1-E_i}\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta\right|\langle x_\alpha^2\rangle\ , \quad \text{(A5b)}$$

where E_1 is the energy of the state closest in energy to the state $|i\rangle$ that contributes to the sum (A4). We can obtain some estimate of the importance of higher-order terms in the expansion in $\delta\mathbf{k}_\alpha$ and $\delta\mathbf{k}_\beta$ from two simple cases where the sum in (A4) can be evaluated by closure.

If the sum is dominated by a single intermediate state,

$$\langle i|T^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)|i\rangle=\frac{t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{E_j-E_i}\times(\langle i|e^{i\delta\mathbf{k}_\alpha\cdot\mathbf{x}}|i\rangle\langle i|e^{i\delta\mathbf{k}_\beta\cdot\mathbf{x}}|i\rangle-\langle i|e^{i(\delta\mathbf{k}_\alpha+\delta\mathbf{k}_\beta)\cdot\mathbf{x}}|i\rangle)\approx\frac{2t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{E_j-E_i}\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta\langle x_\alpha^2\rangle e^{-[(\delta k_\alpha)^2+(\delta k_\beta)^2]\langle x_\alpha^2\rangle/2}\ . \quad \text{(A6)}$$

If the scatterer is bound in a harmonic potential, and the exponential $e^{i\delta\mathbf{k}_\alpha\cdot\mathbf{x}}$ can be expanded, keeping only the leading term,

$$\langle i|e^{i\delta\mathbf{k}_\alpha\cdot\mathbf{x}}|j\rangle\approx i\delta\mathbf{k}_\alpha\cdot\langle i|\mathbf{x}|j\rangle=\delta\mathbf{k}_\alpha\cdot\frac{\langle i|[H,\mathbf{p}]|j\rangle}{M\hbar\omega^2}=\langle i|\delta\mathbf{k}_\alpha\cdot\mathbf{p}|j\rangle\frac{E_i-E_j}{M\hbar\omega^2}\ , \quad \text{(A7)}$$

where H denotes the oscillator Hamiltonian of the scatterer $\mathbf{p}$ its momentum and ω its angular frequency. Substituting (A7) into (A4), summing over the intermediate state by closure and summing over all values of the two momentum transfers gives

$$\sum_{\delta k_\alpha,\delta k_\beta} \langle i|T^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)|i\rangle \approx \sum_{\delta k_\alpha,\delta k_\beta} \frac{t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{M\hbar\omega^2}\langle i|[\delta\mathbf{k}_\alpha\cdot\mathbf{p},e^{i\delta\mathbf{k}_\beta\cdot\mathbf{x}}]|i\rangle$$
$$= \sum_{\delta k_\alpha,\delta k_\beta} \frac{t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta}{M\omega^2}\langle i|e^{i\delta\mathbf{k}_\beta\cdot\mathbf{x}}|i\rangle$$
$$= \sum_{\delta k_\alpha,\delta k_\beta} \frac{2t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{(2n+1)\hbar\omega}\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta\langle x_\alpha^2\rangle\langle i|e^{i\delta\mathbf{k}_\beta\cdot\mathbf{x}}|i\rangle , \qquad \text{(A8a)}$$

where $\langle x_\alpha^2\rangle=(2n+1)\hbar/2M\omega$. The matrix element on the right-hand side is just a Debye-Waller factor for the momentum transfer δk_β. The approximation (A7) which is good only to first order in δk_α but good to all others in δk_β loses the symmetry between the two momentum transfers of the original expression (A4). We can restore this symmetry by adding an additional Debye-Waller factor for the momentum transfer δk_α which is of higher order in δk_α. Evaluating the matrix element then gives

$$\sum_{\delta k_\alpha,\delta k_\beta} \langle i|T^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)\approx \sum_{\delta k_\alpha,\delta k_\beta} \frac{2t^{(2)}(\mathbf{p}_e,\delta\mathbf{k}_\alpha,\delta\mathbf{k}_\beta)}{(2n+1)\hbar\omega}\cdot\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta\langle x^2\rangle e^{-[(\delta k_\alpha)^2+(\delta k_\beta)^2]\langle x_\alpha^2\rangle/2} . \qquad \text{(A8b)}$$

Note that this result (A8b) reduces to the previous case (A6) for $n=0$, where only a single intermediate state contributes to the sum (A4), and both (A6) and (A8) reduce to (A5b) to lowest order in $\delta\mathbf{k}_\alpha$ and $\delta\mathbf{k}_\beta$.

The first factor on the right-hand sides of Eqs. (A4), (A6), and (A8) involves ratios of some energy characteristic of the scattering interaction to the energy-level spacing of the scatterer. These factors are small if the Born approximation is valid for the scattering. The remaining factors include Debye-Waller factors which are of order unity if the probability for single elastic scattering is appreciable. Thus corrections to the Born approximation contain the same Debye-Waller factors for somewhat different momentum transfers, but do not qualitatively change the previous result that the simple description with elastic coherence is valid whenever the relevant Debye-Waller factors are of order unity; i.e., the probability of inelastic scattering is not large. The entire second-order contribution is seen to be small if the Debye-Waller factor is near unity, even if the first factor is comparable to the first-order result (A3) and the Born approximation breaks down. The expressions (A5)–(A8) all contain the small factor $\delta\mathbf{k}_\alpha\cdot\delta\mathbf{k}_\beta\langle x_\alpha^2\rangle$.

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