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Appendices

Appendix A: The Scatterer Potential

In the present work, we assume that each scatterer potential has a Gaussian form

$$v_1\left(\mathbf{x}-\mathbf{x}_i'\right)=v_0\exp\left[-\frac{\left|\mathbf{x}-\mathbf{x}_i'\right|^2}{l_0^2}\right]. \tag{A.1}$$

where v_0 is strength of the scatterer potential. We expect that the potential of a double scatterer (the two adjacent scatterers) will have as equal height as that of a single scatterer, as a result, the potential of a single scatterer at $a_0/2$, the middle point between centers of the two scatterers must have only half height in order to overlap each other and create the same height. Thus we can find

$$l_0=\frac{a_0}{2\sqrt{\ln 2}}, \tag{A.2}$$

where a_0 is the atomic nearest neighbor distance in crystalline silicon. Substituting in eq.(A.1), the scatterer potential becomes

$$v_1\left(\mathbf{x}-\mathbf{x}_i'\right)=v_0\exp\left[-\frac{4\ln 2}{a_0^2}\left|\mathbf{x}-\mathbf{x}_i'\right|^2\right]. \tag{A.3}$$

Appendix B: Mathematical Properties of Path Integral with Quadratic Action

The simplest path integrals are those in which all exponent of the variables are up to the second degree. Consider a particle whose Lagrangian is in the form as follows

$$L(\dot{\mathbf{x}}, \mathbf{x}; t) = a(t)\,\dot{\mathbf{x}}^2 + b(t)\,\dot{\mathbf{x}}\cdot\mathbf{x} + c(t)\,\mathbf{x}^2 + d(t)\,\dot{\mathbf{x}} + e(t)\,\mathbf{x} + \mathbf{f}(t). \tag{B.1}$$

We need to determine

$$K(a,b) = \int_a^b D(\mathbf{x}(t)) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} L(\dot{\mathbf{x}}, \mathbf{x}; t)\, dt\right], \tag{B.2}$$

the integral over all paths from $(\mathbf{x}_a, t_a)$ to $(\mathbf{x}_b, t_b)$. Primarily, it is noted that the form of the Lagrangian is too general for our determination. Since we are concerned only with (B.2), we could remove the factor $\dot{\mathbf{x}}$ from those terms in which it is linear through an integration by parts.

If we signify $\mathbf{x}_c(t)$ as the classical path between the specified end points, then $\mathbf{x}_c$ is an extremum for the action S, and we write $S_{cl}[b,a] = S[\mathbf{x}_c(t)]$. Then, the variable $\mathbf{x}$ in (B.2) can be changed by

$$\mathbf{x} = \mathbf{x}_c + \mathbf{y}. \tag{B.3}$$

This means that, instead of defining a point on the path by its distance $\mathbf{x}(t)$ from an arbitrary coordinate axis, we measure instead the deviation $\mathbf{y}(t)$ from the classical path $\mathbf{x}_c(t)$ and hence $D(\mathbf{x}(t)) = D(\mathbf{y}(t))$. The action becomes

$$\begin{aligned} S[\mathbf{x}(t)] &= S[\mathbf{x}_c(t) + \mathbf{y}(t)] \\ &= \int_{t_a}^{t_b} \left[a(t)\left(\dot{\mathbf{x}}_c^2 + 2\dot{\mathbf{x}}_c\dot{\mathbf{y}} + \dot{\mathbf{y}}^2\right) + ...\right] dt. \end{aligned} \tag{B.4}$$

Since $\mathbf{x}_c$ is so chosen leading to no change in S, to first order, for the variations of the path around $\mathbf{x}_c$, all terms that contain $\mathbf{y}$ as a linear are factor cancelled, and the remaining are the second-order term in $\mathbf{y}$. Thus (B.4) can be written as

$$S[\mathbf{x}(t)] = S_{cl}[b, a] + \int_{t_a}^{t_b} \left[a(t)\left(\dot{\mathbf{y}}_c^2 + b(t)\, 2\dot{\mathbf{y}} \cdot \mathbf{y} + c(t)\, \mathbf{y}^2\right)\right] dt, \tag{B.5}$$

and the propagator reduces to

$$K(b, a) = \exp\left\{\frac{i}{\hbar} S_{cl}[b, a]\right\} \int_0^0 D(\mathbf{y}(t)) \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} \left[a(t)\left(\dot{\mathbf{y}}_c^2 + b(t)\, 2\dot{\mathbf{y}} \cdot \mathbf{y} + c(t)\, \mathbf{y}^2\right)\right]\right]. \tag{B.6}$$

Since all path $\mathbf{y}(t)$ start from and return to the point that $\mathbf{y} = 0$, the integral over paths is a function of the times at the end points only, and therefore

$$K(b, a) = \exp\left\{\frac{i}{\hbar} S_{cl}[b, a]\right\} F(t_a, t_b). \tag{B.7}$$

The dependence upon the spatial variables $\mathbf{x}_a$ and $\mathbf{x}_b$ is completely determined. The factor $F(t_a, t_b)$ must be determined by some other property of the solution or by evaluation through Fourier series expansion (Feynman and Hibbs, 1965).

Here, we consider the average $\langle ... \rangle_0$ of a functional A by a quadratic action S_0, which is defined as

$$\langle A \rangle_0 = \frac{\int D(\mathbf{x}(\tau))\; A\; \exp\left[\frac{i}{\hbar} S_0\right]}{\int D(\mathbf{x}(\tau)) \exp\left[\frac{i}{\hbar} S_0\right]}. \tag{B.8}$$

If we choose for the functional A the particular form

$$A = \exp\left[\frac{i}{\hbar}\int d\tau\ \mathbf{f}(\tau)\cdot x(\tau)\right], \tag{B.9}$$

then the numerator shows an action $S^f = S + \int d\tau\ \mathbf{f}(\tau)\cdot x(\tau)$, which is clearly quadratic. Thus the numerator path integral can be carried out as described above, so that

$$\int_a^b D(\mathbf{x}(\tau))\exp\left[\frac{i}{\hbar}S^f\right] = \exp\left[\frac{i}{\hbar}S^f_{cl}[b,a]\right]F'(t_a,t_b). \tag{B.10}$$

The integral over the path $\mathbf{y}$, $F'(t_a,t_b)$ is independent on the function $\mathbf{f}(t)$, because this function appears in the action $S^{f\prime}$ multiplying only a linear term in $\mathbf{x}(t)$ and, from (B.6), $F'(t_a,t_b)$ composes only quadratic parts of $S^{f\prime}$. Hence $F'(t_a,t_b) = F(t_a,t_b)$, which implies that

$$\left\langle \exp\left[\frac{i}{\hbar}\int d\tau\ \mathbf{f}(\tau)\cdot x(\tau)\right]\right\rangle_0 = \exp\left[\frac{i}{\hbar}\left\{S^f_{cl}[b,a] - S_{cl}[b,a]\right\}\right]. \tag{B.11}$$

Once the classical action $S'_{cl}[b,a]$ has been obtained, $S_{cl}[b,a]$ can be found by simply setting $\mathbf{f}(\tau)\equiv 0$. Suppose we take the functional derivative with respect to $\mathbf{f}(\tau)$ to (B.11) to get

$$\begin{aligned}\left\langle \mathbf{x}(\tau)\exp\left[\frac{i}{\hbar}\int d\tau\ \mathbf{f}(\tau)\cdot x(\tau)\right]\right\rangle_0 &= \frac{\hbar}{i}\frac{\delta}{\delta\mathbf{f}(\tau)}\left[\exp\left[\frac{i}{\hbar}\left(S^f_{cl}[b,a] - S_{cl}[b,a]\right)\right]\right] \\ &= \frac{\delta}{\delta\mathbf{f}(\tau)}S^f_{cl}[b,a] \\ &\quad\cdot\left[\exp\left[\frac{i}{\hbar}\left(S^f_{cl}[b,a] - S_{cl}[b,a]\right)\right]\right].\end{aligned} \tag{B.12}$$

Evaluating both sides when $\mathbf{f}(\tau)\equiv 0$, we obtain

$$\langle\mathbf{x}(\tau)\rangle_0 = \left.\frac{\delta}{\delta\mathbf{f}(\tau)}S^f_{cl}[b,a]\right|_{\mathbf{f}(\tau)\equiv 0}. \tag{B.13}$$

we can continue this process to get the second derivative,

$$\langle \mathbf{x}(\tau) \cdot \mathbf{x}(\sigma) \rangle_0 = \frac{\hbar}{i} \left[\frac{\delta^2 S_{cl}^f}{\delta \mathbf{f}(\tau)\, \delta \mathbf{f}(\sigma)} + \frac{\delta S_{cl}^f}{\delta \mathbf{f}(\tau)} \frac{\delta S_{cl}^f}{\delta \mathbf{f}(\tau)} \right] \Bigg|_{\mathbf{f}(\tau) \equiv 0} . \tag{B.14}$$

Actually, since S^f is quadratic only in $\mathbf{f}$, the average of any number of $\mathbf{x}(\tau)$, $\langle \mathbf{x}(\tau) \cdot \mathbf{x}(\lambda) \cdots \mathbf{x}(\sigma) \rangle_0$, can be directly evaluated in terms of

$$\frac{\delta^2 S_{cl}^f}{\delta \mathbf{f}(\tau)\, \delta \mathbf{f}(\sigma)} \text{ and } \frac{\delta S_{cl}^f}{\delta \mathbf{f}(\tau)}. \tag{B.15}$$

Appendix C: The Harmonic Wave Function

As referred previously in Section 3.3.1, the envelope matrix element of transition described in eq.(3.23) is a function of initial and final state wave functions which may be localized and delocalized. However, in this Appendix, we particularly are involved with localized wave function since the delocalized wave function obviously is plane wave. Anyway, more details of the derivation can be found in Ph.D. Thesis of Wichit Sritrakool (1984).

According to the Feynman path integration formalism, it well appears that a propagator can imply direct information of the wave function of the system (Feynman and Hibbs, 1965). By the suggestion of Samathiyakanit (1974), the average propagator is exactly appraised up to the first cumulant with the variational parameter arised from the Lloyd and Best variational principle (1975). Such propagator is called the first -order propagator. Although, in principle, we actually should employ the first-order propagator in order to derive the wave function. But, refer to quantum mechanics, it is well known that the zero-order wave function is adequate if the first-order energy is required.

The zero-order propagator achieved by Samathiyakanit (1974) is

$$G_0(\mathbf{x},\mathbf{t}\,;\mathbf{x}',\mathbf{t}') = \left(\frac{m}{2\pi i\hbar\,(t-t')}\right)^{3/2}\left(\frac{\omega t}{2\sin(\omega t/2)}\right)^{3/2} \times \exp\left[\frac{i}{\hbar}\frac{m\omega}{4}\cot(\omega t/2)\,|\mathbf{x}-\mathbf{x}'|^2\right] \tag{C.1}$$

Because this expression is clearly translationally invariant, therefore, information on localized states is unavailable. To get localized wave functions, the translational invariance have to be broken. The idea of breaking the translational symmetry resemble to that used in the mean field theory (Ascroft and Mermin, 1976, for a brief review).

In order to overcome this problem, it should be remarked that eq.(C.1) can be derived by averaging over all directions the propagator of the harmonic oscillator centered at other positions, G_H, i.e.

$$G_0(\mathbf{x}, \mathbf{t}\ ; \mathbf{x}', \mathbf{t}') \sim \int d\mathbf{R}\ G_H(\mathbf{x}+\mathbf{R}, t; \mathbf{x}'+\mathbf{R}, t') . \tag{C.2}$$

where

$$G_H(\mathbf{x}+\mathbf{R}, t; \mathbf{x}'+\mathbf{R}, t') = \int D(\mathbf{x}(\tau)) \exp\left[\frac{i}{\hbar}\int_{t'}^{t} d\tau\ \frac{m}{2}\left(\dot{\mathbf{x}}^2(\tau) - \omega^2(\mathbf{x}(\tau)+\mathbf{R})^2\right)\right] . \tag{C.3}$$

For simplicity, $\mathbf{R} = 0$ is set and the well known result is obtained

$$\begin{aligned} G_H(\mathbf{x}, t; \mathbf{x}', t') &= \left(\frac{m\omega}{2\pi i\hbar \sin\omega(t-t')}\right)^{3/2} \\ &\quad \exp\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t-t')}\left\{\left(\mathbf{x}^2 - \mathbf{x}'^2\right)\cos\omega(t-t') - 2\mathbf{x}\cdot\mathbf{x}'\right\}\right] \\ &= \sum_n \phi_n(\mathbf{x})\,\phi_n^*(\mathbf{x}')\exp\left[-\frac{i}{\hbar}E_n(t-t')\right] \end{aligned} \tag{C.4}$$

where E_n and ϕ_n are harmonic oscillator energies and wave functions respectively. To gain the localized wave function corresponding to the density of states, we have to take the limit t to infinity (Feynman and Hibbs, 1965). Such manipulation corresponds to taking the ground-state wave function only, for example

$$G_H(\mathbf{x}, t; \mathbf{x}', t') \simeq \phi_n(\mathbf{x})\,\phi_n^*(\mathbf{x}')\exp\left[-\frac{i}{\hbar}\frac{\hbar\omega}{2}(t-t')\right] \tag{C.5}$$

where

$$\phi_0(\mathbf{x}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4}\exp\left[-\frac{m\omega\mathbf{x}^2}{2\hbar}\right], \tag{C.6}$$

the parameter ω which is related to z can variationally be examined from eq.(2.100), (2.101) or (2.104). The envelope wave function for a localized state, eq.(C.6), can be rewritten as

$$\phi_0\left(\mathbf{x}\right) = \left(\frac{2\mu}{\pi}\right)^{3/4} \exp\left(-\mu\mathbf{x}^2\right) \tag{C.7}$$

on the basis of the relation

$$\mu = \frac{m\omega}{2\hbar} = \frac{z}{4L^2} \,. \tag{C.8}$$

Vitae

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